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REVIEW ARTICLE

Artificial Intelligence for Sustainable Energy Transition: A Comprehensive Review of Machine Learning, Deep Learning, and Intelligent Optimization Techniques

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Abstract
The global transition toward sustainable energy systems requires advanced technologies capable of improving renewable energy integration, optimizing electricity generation and consumption, and enhancing energy-system reliability. Artificial intelligence (AI) has emerged as an important enabling technology for addressing these challenges through data-driven prediction, intelligent control, and computational optimization. This review examines the contributions of machine learning, deep learning, reinforcement learning, and intelligent optimization techniques to sustainable energy transitions. It explores their applications in renewable energy forecasting, smart-grid management, energy storage, demand-side management, predictive maintenance, and integrated energy systems. Particular attention is given to the complementary capabilities of conventional machine learning algorithms, advanced neural network architectures, hybrid intelligence, and nature-inspired optimization approaches. The review also evaluates important implementation barriers, including data limitations, model interpretability, computational requirements, cybersecurity, algorithmic reliability, and the environmental footprint of AI infrastructure. Emerging opportunities involving explainable AI, physics-informed learning, federated learning, digital twins, and multi-agent intelligent systems are discussed. The review highlights that AI can accelerate energy-system decarbonization by improving operational efficiency, flexibility, and renewable energy utilization, provided that its deployment is supported by transparent governance, reliable data infrastructures, and sustainability-oriented evaluation frameworks.

Keywords: Artificial intelligence; Machine learning; Deep learning; Intelligent optimization; Sustainable energy transition

1. Introduction

The transition toward sustainable energy systems has become a central component of international efforts to address climate change, strengthen energy security, and promote sustainable economic development. Conventional energy systems remain heavily dependent on fossil fuels, contributing substantially to greenhouse gas emissions and environmental degradation. Consequently, governments, industries, and energy-sector stakeholders are increasingly prioritizing renewable energy deployment, energy efficiency, electrification, and low-carbon technological innovation. However, the transition from centralized fossil-fuel-based electricity

systems toward decentralized and renewable-dominated energy infrastructures introduces considerable technical, economic, and operational challenges. Solar photovoltaic (PV) and wind energy technologies have experienced substantial technological development, but their variable generation characteristics create difficulties for electricity forecasting, grid balancing, energy storage, and real-time operational management. Increasing shares of distributed generation, electric vehicles, battery storage, and flexible electricity demand further increase the complexity of modern energy networks. Addressing these challenges requires more sophisticated approaches to forecasting, decision-making, optimization, and system control.

Artificial intelligence (AI) offers considerable potential to support these requirements by transforming large volumes of energy-related data into actionable information. Through machine learning, deep learning, reinforcement learning, and intelligent optimization, AI systems can identify complex relationships, predict energy demand and renewable generation, detect operational abnormalities, and improve the allocation of energy resources. Unlike conventional approaches that frequently depend on predetermined mathematical relationships and operating assumptions, data-driven AI methods can learn from historical observations and adapt to changing operational conditions (Donti and Kolter, 2021). The relevance of AI to sustainable energy systems extends beyond renewable energy prediction. Its applications encompass electricity generation, transmission, distribution, storage, consumption, and energy-market operations. For example, AI-based forecasting can improve the scheduling of wind and solar generation, while intelligent optimization can support economic dispatch, battery management, and demand response. Reinforcement learning can additionally facilitate adaptive control of microgrids and distributed energy resources under uncertain operating conditions. These capabilities have established AI as an increasingly important component of intelligent energy infrastructure (Donti and Kolter, 2021; Li et al., 2024a).

Nevertheless, the relationship between AI and sustainable energy transition is not automatically positive. AI systems depend on data infrastructure, computing resources, communication networks, and electricity consumption. Large-scale deployment may therefore introduce additional energy demand, cybersecurity risks, and environmental impacts. The International Energy Agency (IEA) emphasizes this dual relationship: AI can transform energy-sector operations, while the expansion of AI infrastructure itself creates additional electricity requirements. Although previous studies have investigated individual applications of ML, DL, and optimization in renewable energy forecasting, microgrid management, and smart-grid operation, there remains a need for an integrated perspective connecting these technical approaches with broader sustainable energy outcomes. In particular, understanding the complementary functions of prediction, optimization, and intelligent control is essential for translating AI innovations into practical energy-transition benefits.

Against this background, this review examines the role of AI in accelerating sustainable energy transitions, with particular emphasis on three interconnected technological dimensions: machine learning, deep learning, and intelligent optimization. It synthesizes their major applications across renewable energy systems, smart grids, energy storage, and energy management; evaluates their technical and implementation limitations; and identifies emerging research priorities for developing reliable, efficient, and environmentally responsible AI-enabled energy infrastructure.

2. Artificial intelligence techniques for sustainable energy systems

AI encompasses computational approaches that enable machines to perform tasks involving prediction, pattern recognition, learning, optimization, and decision-making. In sustainable energy systems, these capabilities are particularly relevant because electricity generation, consumption, and distribution are influenced by multiple interacting variables, including meteorological conditions, equipment performance, consumer behavior,

electricity prices, and network constraints. Three major methodological categories are particularly important: conventional machine learning, deep learning, and intelligent optimization. Although these approaches have different computational foundations, their integration can provide more comprehensive solutions to complex energy-management problems.

2.1. Machine learning approaches

Machine learning involves algorithms that identify patterns and relationships within datasets and use these relationships to generate predictions or classifications. Supervised, unsupervised, and semi-supervised learning represent three major learning paradigms relevant to energy applications. Supervised learning is frequently employed for electricity-demand forecasting, renewable energy prediction, equipment-failure detection, and energy-consumption estimation. Algorithms such as support vector machines (SVM), random forests (RF), decision trees, gradient boosting, and artificial neural networks (ANNs) can model nonlinear relationships between energy-system variables. Support vector regression is particularly useful for nonlinear prediction problems involving relatively structured datasets. Random forests combine multiple decision trees and can capture nonlinear interactions while reducing sensitivity to individual training samples. Gradient-boosting algorithms, including XGBoost, can provide effective predictive performance for structured energy datasets containing meteorological, operational, and temporal variables.

Unsupervised learning is useful when labeled observations are unavailable or expensive to obtain. Clustering methods can identify electricity-consumption profiles, classify operational conditions, and group renewable generation patterns. Anomaly-detection approaches can also identify unusual equipment behavior and potentially indicate emerging operational faults. Semi-supervised learning offers an alternative when only a limited proportion of energy observations are labeled. This is relevant to equipment diagnostics and renewable energy infrastructure, where obtaining verified fault records may be difficult.

The principal advantage of conventional ML is its flexibility across different energy-related prediction and classification tasks. Nevertheless, model performance depends on data quality, feature selection, training procedures, and the extent to which historical operating conditions represent future environments. Donti and Kolter (2021) emphasize that the successful use of ML in sustainable energy systems requires consideration of both predictive performance and the physical and operational characteristics of energy infrastructure.

2.2. Deep learning techniques

Deep learning represents an advanced branch of ML that uses multilayer neural networks to learn complex data representations. Its capacity to identify nonlinear relationships and extract features from large datasets makes it particularly useful for energy applications involving time-series observations, spatial information, and high-dimensional sensor measurements. Recurrent neural networks (RNNs) and long short-term memory (LSTM) networks are widely investigated for forecasting applications because they can represent temporal dependencies in sequential data. Their applications include electricity-load prediction, solar radiation estimation, wind-power forecasting, and renewable generation scheduling.

Convolutional neural networks (CNNs) are particularly relevant to extracting spatial and local patterns from image-based or structured data. In solar energy systems, CNNs can analyze sky images and satellite observations to support short-term solar irradiance forecasting. They can also contribute to equipment inspection and fault identification. Gated recurrent units (GRUs) provide an alternative recurrent architecture with a comparatively simplified gating structure. They can be applied to electricity demand and renewable generation forecasting,

particularly when computational efficiency is an important consideration. Transformer architectures have introduced attention-based approaches for modeling relationships across time-series observations. Their ability to represent long-range dependencies has attracted interest in energy forecasting and multivariable energy-management applications. However, their performance should be assessed against simpler baselines, especially when datasets are limited. Graph neural networks (GNNs) are particularly relevant to electricity networks because grid infrastructure can be represented as interconnected nodes and transmission lines. This representation allows the model to consider spatial relationships and network connectivity when analyzing electricity demand, voltage behavior, and power-system operating conditions.

Recent reviews have examined the development of DL architectures for PV forecasting, identifying MLP, RNN, CNN, and GNN approaches among the principal model families (Yu et al., 2024). The main limitation of DL is its dependence on substantial training data and computational resources. Complex architectures may also be difficult to interpret, and high predictive accuracy in historical datasets does not necessarily guarantee reliable performance under changing meteorological or operational conditions.

2.3. Reinforcement learning and adaptive intelligence

Reinforcement learning is a learning paradigm in which an agent interacts with an environment and learns decision-making strategies through rewards and penalties. Rather than relying exclusively on labeled training examples, an RL agent evaluates the consequences of its actions and progressively improves its policy. This approach is relevant to energy systems because many operational decisions involve sequential choices under uncertainty. Examples include battery charging and discharging, electricity trading, flexible demand scheduling, microgrid operation, and real-time energy dispatch.

Deep reinforcement learning combines RL with neural networks to manage environments with large or continuous state spaces. Algorithms such as deep Q-networks (DQN), deep deterministic policy gradients (DDPG), proximal policy optimization (PPO), and soft actor-critic (SAC) have been investigated for energy-control applications. Dinata et al. (2024) reviewed the application of deep reinforcement learning to microgrid control and highlighted its potential for adaptive energy management and renewable energy integration. Similarly, studies of home energy management have investigated RL-based approaches for demand response, appliance scheduling, and renewable energy utilization (Latoń et al., 2024).

Despite these opportunities, RL requires careful consideration of exploration risks, reward-function design, training stability, and operational safety. In real electricity networks, unrestricted exploration can produce unacceptable control actions. Consequently, simulation environments, digital twins, constrained policies, and human-supervised deployment are important components of responsible RL implementation.

2.4. Intelligent optimization and hybrid AI approaches

Intelligent optimization refers to computational techniques designed to identify effective solutions to complex optimization problems, particularly when conventional mathematical methods encounter nonlinearities, multiple objectives, or large search spaces. Genetic algorithms (GA), particle swarm optimization (PSO), ant colony optimization (ACO), differential evolution (DE), and other evolutionary or swarm-intelligence methods have been investigated in renewable energy system design, microgrid scheduling, economic dispatch, and energy-resource allocation.

Genetic algorithms employ selection, crossover, and mutation to evolve candidate solutions. PSO uses interactions among particles to search for promising regions of an optimization space. These approaches can

support the sizing of hybrid renewable energy systems, battery allocation, and optimal operating strategies. Hybrid AI approaches combine different computational methods to exploit their complementary capabilities. For example, an LSTM model may forecast solar generation, while PSO optimizes battery scheduling using the predicted output. Similarly, a machine-learning model may estimate electricity demand before an optimization algorithm determines an appropriate generation and storage schedule.

It is important to distinguish predictive learning from optimization. ML and DL generally estimate unknown relationships or future system states, whereas optimization methods identify decisions that perform well against specified objectives and constraints. Their integration therefore provides a useful framework for energy-system intelligence. Table 1 summarizes the major AI techniques, their capabilities, and their relevance to sustainable energy systems. Figure 1 presents the conceptual relationship between AI methodologies, energy-system applications, and sustainability outcomes.

Table 1. Major artificial intelligence techniques for sustainable energy systems: principles, capabilities, and applications

AI technique	Representative algorithms	Principal capabilities	Major energy applications
Supervised ML	SVM, RF, XGBoost, ANN	Prediction and classification	Solar and wind forecasting, load prediction, fault detection
Unsupervised ML	K-means, hierarchical clustering, autoencoders	Pattern discovery and anomaly detection	Consumer segmentation, operational monitoring
Semi-supervised ML	Pseudo-labeling, self-training	Learning from limited labeled data	Equipment diagnostics, energy classification
Deep learning	CNN, RNN, LSTM, GRU	Complex nonlinear and temporal representation	Renewable forecasting, image analysis, load prediction
Transformer-based learning	Attention-based architectures	Long-range temporal relationships	Multihorizon energy forecasting
Graph neural networks	GCN, GAT	Spatial and network-structured learning	Smart-grid monitoring and network analysis
Reinforcement learning	Q-learning, DQN, PPO, SAC	Sequential adaptive decision-making	Microgrid control, battery scheduling, demand response
Evolutionary optimization	GA, DE	Global and multiobjective search	Renewable-system sizing and economic dispatch
Swarm intelligence	PSO, ACO	Population-based optimization	Hybrid energy-system configuration and scheduling
Hybrid AI	LSTM–PSO, ANN–GA, RL–optimization	Integrated prediction and decision-making	Intelligent energy management and renewable integration

Source: Synthesized from Donti and Kolter (2021) and Li et al. (2024a)

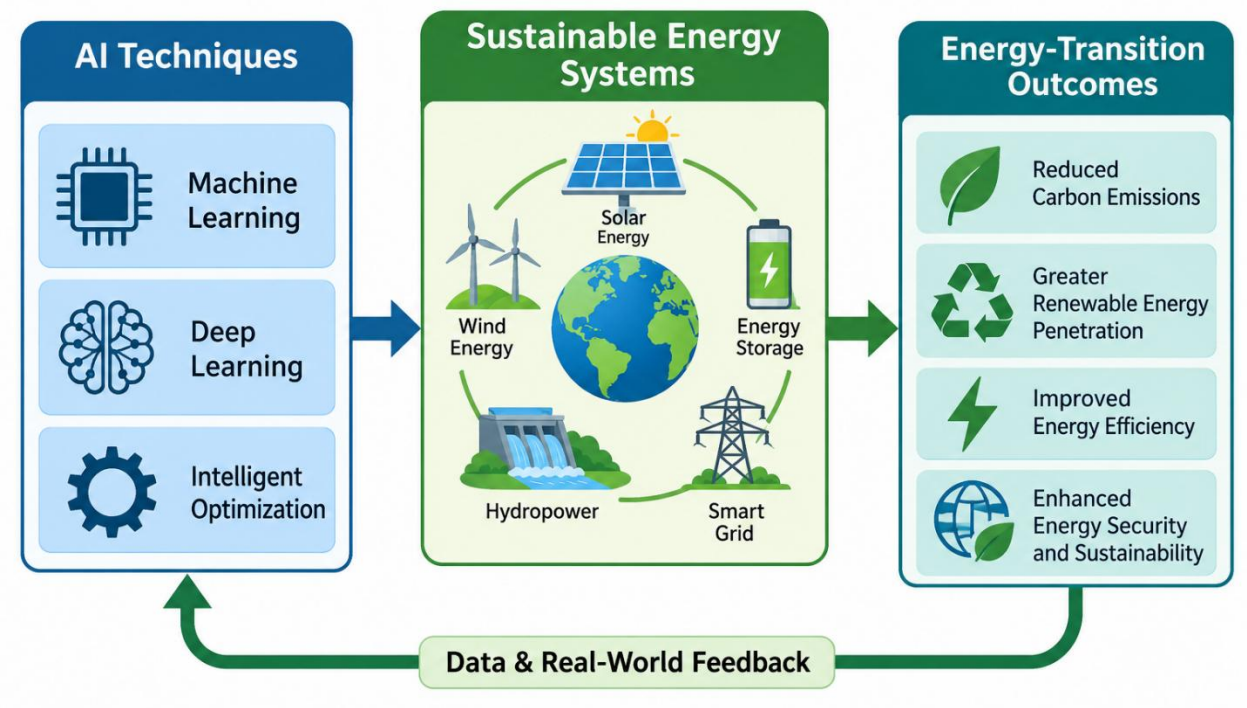

Figure 1. Integrated conceptual framework linking artificial intelligence techniques, sustainable energy systems, and energy-transition outcomes

3. Applications of AI in the sustainable energy transition

The sustainable energy transition requires improvements across the entire energy value chain, including generation, transmission, distribution, storage, and consumption. AI can support these improvements by combining predictive analytics, automated decision-making, and intelligent resource allocation. Its applications are particularly important in renewable energy systems, where variable generation and distributed electricity resources create additional operational complexity.

3.1. Renewable energy generation forecasting

Accurate renewable energy forecasting is one of the most established applications of AI in sustainable energy systems. Solar and wind generation depend on meteorological variables, including temperature, solar irradiance, wind speed, atmospheric pressure, humidity, and cloud cover. Their variability creates uncertainty in electricity generation and complicates grid balancing. In solar energy systems, ML algorithms such as RF, SVM, ANN, and gradient boosting have been used to estimate solar irradiance and PV power production. These models can incorporate historical electricity generation, meteorological measurements, satellite observations, and numerical weather prediction data. DL models have expanded forecasting capabilities by learning complex temporal and spatial relationships. LSTM and GRU architectures are frequently investigated for short-term and day-ahead PV forecasting, while CNN models can extract useful information from satellite images and sky-camera observations. Barhmi et al. (2024) reviewed solar forecasting approaches and emphasized the importance of forecasting horizons, meteorological inputs, preprocessing, and model selection. Another review of PV forecasting identified the diversity of ML techniques and the need for more consistent comparisons across datasets and operating environments (Alcañiz et al., 2023). Wind energy forecasting presents similar opportunities. ML models can

analyze historical turbine performance, wind speed, direction, air density, and weather forecasts to estimate future power output. Yang et al. (2024) reviewed ML-based wind forecasting and discussed the development of different approaches for addressing the variability and uncertainty of wind generation.

A critical distinction is the forecasting horizon. Very-short-term forecasting supports real-time control, short-term forecasting facilitates operational scheduling, and medium- or long-term forecasting supports electricity trading, maintenance planning, and infrastructure development. Consequently, the most appropriate model depends on the intended operational decision rather than predictive accuracy alone. The use of probabilistic forecasting is also important. Instead of providing only a single predicted value, AI models can estimate prediction intervals, quantiles, or probability distributions. Such outputs allow system operators to consider forecast uncertainty when scheduling reserves and allocating storage resources.

3.2. Smart grids and intelligent electricity management

Smart grids represent a fundamental component of the sustainable energy transition because they facilitate bidirectional electricity flows, distributed generation, advanced metering, automated control, and real-time communication. Traditional electricity networks were primarily designed around centralized generation and predictable consumption patterns. However, increasing penetration of rooftop PV, wind farms, battery storage, and electric vehicles requires more flexible electricity management.

AI can improve smart-grid operations through electricity-demand forecasting, voltage monitoring, fault identification, congestion management, and adaptive power-flow control. For example, supervised ML models can predict electricity demand using historical consumption, weather conditions, calendar variables, and socioeconomic indicators. DL architectures can identify complex temporal relationships in high-frequency smart-meter datasets. These capabilities are particularly relevant to distribution networks experiencing rapid changes in electricity consumption. GNNs offer additional opportunities because electricity grids have a naturally interconnected structure. By representing substations, generators, consumers, and transmission lines as network components, graph-based models can incorporate spatial relationships when predicting grid conditions.

AI can also support automated fault detection and system restoration. Models trained on historical operational measurements can identify abnormal voltage, frequency, and equipment behavior. Such capabilities can help operators prioritize maintenance and respond more effectively to emerging network problems. Judge et al. (2024) examined AI approaches for smart-grid integration and optimization, highlighting the relevance of intelligent and nature-inspired techniques for managing increasingly complex electricity networks. Nevertheless, AI-based grid management should complement rather than replace established power-system engineering principles. Voltage stability, frequency response, thermal limits, protection coordination, and network security must remain explicit constraints in intelligent control systems.

3.3. Energy storage and intelligent battery management

Energy storage is essential for balancing variable renewable generation and electricity demand. Battery energy storage systems can absorb surplus electricity during periods of high renewable generation and release electricity when generation is insufficient. AI can improve battery management by estimating state of charge (SOC), state of health (SOH), remaining useful life, degradation characteristics, and optimal charging and discharging schedules. SOC estimation determines the available stored energy, whereas SOH estimation evaluates battery condition relative to its original performance. Both are important for operational safety, asset management, and storage-system longevity. ML algorithms, including SVM, RF, ANN, and Gaussian process regression, have been

investigated for SOC and SOH estimation. DL architectures can additionally identify nonlinear degradation patterns from voltage, current, temperature, and cycling measurements. Ren and Du (2023) examined ML-based SOC and SOH estimation, including neural networks, DL, SVM, and Gaussian process regression. The review highlighted the importance of datasets, input-feature selection, model parameters, and performance evaluation.

AI-based battery management can also improve operational scheduling. For example, reinforcement learning can determine charging and discharging actions based on electricity prices, renewable generation, battery condition, and anticipated demand. However, optimization should account for battery degradation rather than focusing exclusively on short-term electricity costs. Frequent cycling, excessive charging rates, and unfavorable operating temperatures can accelerate degradation and reduce storage-system lifetime. Consequently, intelligent battery management should integrate operational efficiency, degradation-aware scheduling, safety constraints, and lifecycle considerations.

3.4. Demand response and energy efficiency

Demand response involves modifying electricity consumption in response to grid requirements, electricity prices, or renewable generation availability. It is particularly important in electricity systems with high shares of variable renewable energy. AI can facilitate demand response by forecasting consumption patterns and identifying opportunities for flexible electricity use. Residential, commercial, and industrial consumers can potentially adjust the timing of electricity consumption without compromising essential energy services.

In residential buildings, AI-based home energy management systems can coordinate heating, ventilation, air conditioning, lighting, appliances, rooftop PV, and battery storage. RL approaches are particularly relevant because they can learn scheduling policies that balance electricity expenditure, occupant comfort, and renewable energy utilization. Latoń et al. (2024) reviewed the application of deep reinforcement learning to home energy management, including demand response, load scheduling, and renewable energy integration.

In commercial buildings, ML can predict occupancy-related energy requirements and optimize heating and cooling operations. In industrial facilities, intelligent algorithms can identify energy-intensive processes and recommend operational adjustments. Energy efficiency improvements should also consider the rebound effect, whereby lower operating costs may encourage additional energy consumption. Therefore, AI-enabled efficiency initiatives should be evaluated using actual energy savings rather than algorithmic performance alone.

3.5. Predictive maintenance and operational reliability

Renewable energy infrastructure requires continuous monitoring to maintain reliable operation. Wind turbines, solar PV installations, transformers, inverters, and battery systems are exposed to operational stress and environmental conditions that can lead to equipment deterioration. Conventional maintenance strategies often rely on scheduled inspections or reactive repairs. Predictive maintenance provides an alternative by using operational data to identify potential equipment failures before they occur. AI models can analyze vibration signals, temperature measurements, electrical characteristics, acoustic observations, and supervisory control and data acquisition (SCADA) records to detect abnormal equipment behavior.

In wind turbines, ML techniques have been investigated for identifying gearbox faults, bearing deterioration, blade damage, and generator abnormalities. A review by recent wind-turbine researchers (2023) examined ML approaches for fault detection, diagnosis, and prognosis, emphasizing the value of condition monitoring for operational reliability. For solar PV systems, AI can identify abnormal generation patterns associated with shading, module degradation, inverter failures, and electrical faults. Predictive maintenance can potentially reduce

unexpected downtime, maintenance costs, and unnecessary replacement of equipment. Nevertheless, its practical effectiveness depends on reliable sensor infrastructure, representative fault datasets, and appropriate integration with existing maintenance procedures.

3.6. Microgrids and distributed energy resources

Microgrids are localized electricity systems that integrate distributed generation, storage, and controllable loads. They can operate in coordination with the main grid or independently under islanded conditions. AI can improve microgrid operation by forecasting generation and demand, coordinating distributed resources, managing battery storage, and optimizing electricity exchange. ML models can predict local electricity demand and renewable generation, while optimization algorithms can determine suitable operating schedules. RL provides an additional mechanism for adaptive control under changing supply and demand conditions.

Dinata et al. (2024) identified deep reinforcement learning as a promising approach for microgrid control, particularly in environments characterized by renewable intermittency and operational uncertainty. Research on community microgrid energy management has also demonstrated the relevance of DRL for coordinating multiple devices and balancing operator objectives with user comfort (Li et al., 2024b). AI-enabled microgrids are especially relevant to remote communities, industrial facilities, university campuses, and geographically isolated electricity systems. Their benefits, however, depend on appropriate system sizing, local resource availability, economic feasibility, and reliable control infrastructure.

3.7. Electric vehicles and vehicle-to-grid integration

Electric vehicles (EVs) are an increasingly important component of sustainable energy transitions. Their integration creates new electricity demand but also introduces opportunities for flexible storage and distributed energy management. AI can support EV charging through demand forecasting, charging-station allocation, battery management, and intelligent charging schedules. By considering electricity prices, renewable generation, grid congestion, and user requirements, AI systems can determine when and where charging should occur. Vehicle-to-grid (V2G) systems enable bidirectional electricity exchange between EV batteries and the electricity network. In principle, aggregated EV fleets can provide flexibility, frequency regulation, and additional storage capacity.

RL and optimization methods are relevant to coordinating EV charging and discharging across multiple vehicles while considering battery degradation and mobility requirements. However, practical V2G implementation requires appropriate charging infrastructure, communication standards, user participation, market arrangements, and battery warranty considerations. AI-based charging optimization cannot independently overcome these institutional and infrastructure limitations.

3.8. AI for hydrogen and integrated low-carbon energy systems

Hydrogen technologies are receiving increasing attention as potential components of low-carbon energy systems, particularly for industrial applications, energy storage, and sectors that are difficult to electrify directly. AI can support hydrogen production through the optimization of electrolyzer operating conditions, electricity consumption, system efficiency, and renewable electricity integration. ML models can predict hydrogen production and equipment performance under varying operating conditions. Intelligent optimization can coordinate renewable electricity availability with electrolyzer operation and hydrogen storage requirements.

AI can also support the integration of electricity, heating, cooling, hydrogen, and transportation within multi-energy systems. These systems require coordinated decision-making across different energy carriers and conversion technologies. The use of AI in integrated energy systems therefore extends the concept of intelligent electricity management toward broader energy-system optimization.

Table 2 summarizes the principal AI applications across renewable energy and associated infrastructure. Figure 2 illustrates how these applications connect to improved energy-system performance and sustainability outcomes.

Table 2. Applications of machine learning, deep learning, and intelligent optimization across renewable and sustainable energy systems

Application area	Relevant AI techniques	Main functions	Expected sustainability contribution
Solar energy	RF, SVM, LSTM, CNN, XGBoost	Irradiance and PV forecasting	Improved solar integration and reduced balancing uncertainty
Wind energy	ANN, LSTM, GRU, ensemble learning	Wind-power forecasting and condition monitoring	Improved generation reliability
Smart grids	ML, GNN, DL, RL	Load forecasting, fault detection, grid control	Improved grid flexibility and reliability
Energy storage	ANN, SVM, GPR, RL, PSO	SOC/SOH estimation and charging optimization	Improved storage utilization and battery management
Demand response	RL, DL, RF	Load prediction and flexible scheduling	Reduced peak demand and improved energy efficiency
Buildings	ANN, LSTM, RL	HVAC and appliance management	Reduced building energy consumption
Predictive maintenance	RF, SVM, CNN, autoencoders	Fault detection and equipment diagnostics	Reduced downtime and maintenance waste
Microgrids	DRL, GA, PSO, hybrid AI	Energy dispatch and resource coordination	Improved renewable integration and resilience
Electric vehicles	RL, optimization, ML	Charging and V2G coordination	Improved charging flexibility
Hydrogen systems	ML, ANN, optimization	Electrolyzer operation and production forecasting	Improved renewable hydrogen integration

4. AI-enabled energy system optimization and smart energy management

Although forecasting and pattern recognition are important AI applications, their greatest practical value often emerges when predictive information is integrated into energy-system optimization and operational decision-making.

Energy systems involve numerous interacting objectives, including minimizing operating costs, reducing emissions, maximizing renewable energy utilization, maintaining supply reliability, and satisfying technical constraints. These objectives may conflict, requiring optimization frameworks capable of evaluating trade-offs.

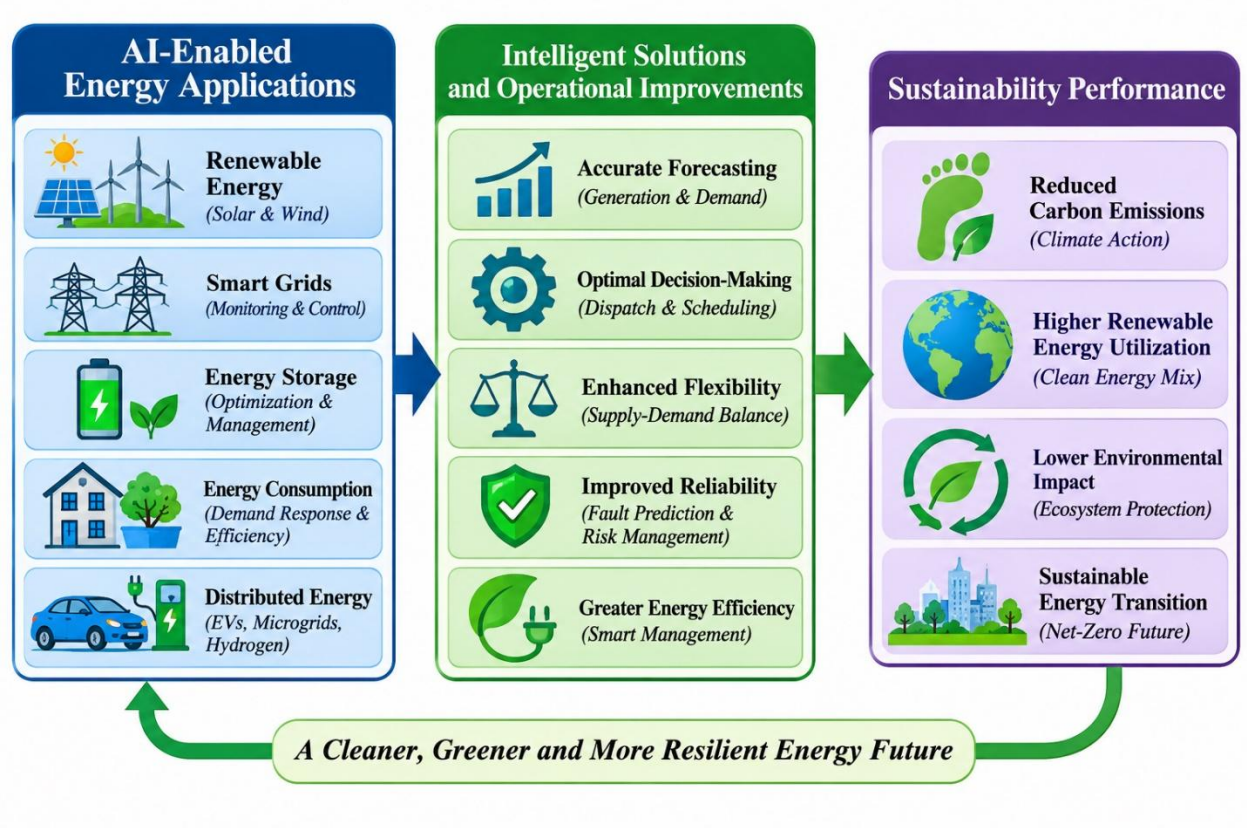

Figure 2. AI-enabled pathways for improving renewable energy integration, energy efficiency, system flexibility, and sustainability performance

4.1. Economic dispatch and optimal power flow

Economic dispatch determines the allocation of electricity generation among available generating units while satisfying electricity demand and operational constraints. Optimal power flow extends this concept by incorporating network conditions, voltage constraints, transmission losses, and other electrical operating requirements. Conventional optimization approaches, including linear programming, nonlinear programming, and mixed-integer optimization, remain important for solving these problems.

AI can complement conventional optimization by estimating uncertain inputs, identifying promising solutions, and accelerating computationally intensive processes. For example, ML models can predict renewable generation and electricity demand before an optimization algorithm determines generation schedules. Similarly, intelligent optimization techniques such as GA and PSO can explore complex solution spaces associated with nonlinear operating constraints.

RL has also been investigated for economic dispatch and operational planning. Wybicki et al. (2024) reviewed RL applications in power-system operation and expansion planning, including economic dispatch, optimal power flow, and network expansion. However, AI-based optimization should not be assumed to outperform mathematical optimization under all conditions. Its suitability depends on the problem structure, computational requirements, solution quality, and ability to respect operational constraints.

4.2. Multiobjective optimization for sustainable energy planning

Sustainable energy planning involves multiple objectives that cannot always be represented by a single economic indicator. For example, an energy system may seek to minimize electricity costs and carbon emissions while maximizing renewable energy utilization and system reliability. Multiobjective optimization can identify a set of alternative solutions representing different trade-offs among competing objectives. Pareto-based approaches are particularly useful for understanding these relationships.

GA, NSGA-II, PSO, and hybrid optimization techniques can be employed to investigate energy-system configurations and operational strategies. These approaches are relevant to hybrid renewable energy systems involving solar PV, wind turbines, batteries, and backup generation. They can also support the optimal sizing and placement of distributed energy resources. Nevertheless, the environmental objectives used in optimization should reflect actual lifecycle impacts. A solution that reduces operational emissions may still have substantial environmental burdens associated with equipment manufacturing, mineral extraction, transportation, and disposal.

4.3. Predictive control and intelligent energy management

Model predictive control (MPC) is an established approach for optimizing system operation over a moving prediction horizon. It uses a system model to estimate future behavior and determine appropriate control actions. AI can enhance MPC by improving forecasts, estimating uncertain parameters, and developing more representative system models. For example, an ML model can predict solar generation and building electricity demand, while MPC determines battery charging, cooling schedules, and grid electricity purchases. Hybrid AI–MPC frameworks are particularly attractive because they combine data-driven prediction with explicit operational constraints. Such frameworks may provide a useful alternative to fully autonomous black-box control in safety-critical energy applications.

4.4. Integrated energy management and sector coupling

Sector coupling involves linking electricity with heating, cooling, transport, and industrial energy systems. It can improve flexibility by allowing energy to be transferred or stored in different forms. AI can support coordinated operation across these systems by forecasting energy requirements, managing conversion technologies, and optimizing resource allocation. For instance, electricity generated during periods of high solar availability can be directed toward battery charging, thermal storage, or hydrogen production, depending on system requirements and economic conditions. An integrated AI-enabled energy management system can therefore coordinate multiple energy resources while considering cost, emissions, storage limitations, and operational constraints. However, practical implementation requires interoperable communication systems, compatible data infrastructures, and coordinated institutional arrangements.

5. Challenges, limitations, and implementation barriers

Despite its considerable potential, AI adoption in sustainable energy systems faces technical, economic, environmental, and institutional barriers (Table 3). These limitations influence model reliability, implementation costs, scalability, and the extent to which AI can contribute to measurable sustainability improvements.

Table 3. Key challenges, limitations, and potential solutions for AI-driven sustainable energy transition

Major challenge	Potential consequences	Recommended solutions
Data scarcity and poor quality	Unreliable predictions and weak generalization	Standardized datasets, data-quality control, data sharing
Limited interpretability	Reduced operational trust	Explainable AI and interpretable models
Computational intensity	Higher costs and additional electricity consumption	Efficient architectures, edge AI, model compression
Cybersecurity threats	Data manipulation and operational disruption	Secure communication, authentication, adversarial testing
Data privacy concerns	Reduced willingness to share operational data	Federated learning and privacy-preserving analytics
Model uncertainty	Unsafe or suboptimal operational decisions	Probabilistic forecasting and uncertainty quantification
Limited scalability	Poor performance across different sites	Transfer learning, domain adaptation, benchmarking
Environmental footprint	Additional lifecycle impacts	Green AI, lifecycle assessment, renewable-powered computing
Skills and institutional barriers	Slow implementation and limited adoption	Workforce development and institutional collaboration
Regulatory uncertainty	Deployment and accountability challenges	Standards, governance frameworks, human oversight

5.1. Data availability, quality, and representativeness

AI models depend on reliable data for training, validation, and operational deployment. However, energy datasets may contain missing observations, measurement errors, inconsistent sampling intervals, sensor failures, and insufficient representation of extreme operating conditions. Renewable energy forecasting is particularly sensitive to data quality because meteorological variability can substantially influence generation. A model trained using data from one geographic location or climatic region may not perform reliably in another.

The availability of high-quality fault datasets is another important challenge for predictive maintenance. Equipment failures are relatively uncommon, and operational datasets may contain many more normal observations than abnormal ones. Data imbalance can therefore produce misleadingly high classification accuracy while failing to identify important faults. Standardized datasets, transparent preprocessing procedures, consistent validation methods, and cross-site benchmarking are necessary to improve the reliability of AI research.

5.2. Model interpretability and operational trust

Many advanced DL and RL approaches operate as complex models whose internal decision-making processes are difficult to interpret. This limitation becomes particularly important in electricity infrastructure, where incorrect decisions can affect grid stability, equipment safety, and energy security. Explainable AI (XAI) approaches, including feature importance, SHAP values, LIME, and interpretable surrogate models, can help explain the relationships underlying model predictions.

However, explanations should be evaluated carefully. A visually understandable explanation does not necessarily establish that a model is physically correct or operationally reliable. Physics-informed machine learning

represents another promising direction because it incorporates physical laws, engineering constraints, or domain knowledge into model development. Such integration can help reduce physically unrealistic predictions and improve model generalization.

5.3. Computational requirements and economic feasibility

Advanced DL and RL models may require substantial computational resources for training, hyperparameter optimization, and continuous operation. These requirements can increase implementation costs and electricity consumption, particularly when large-scale models are deployed across multiple energy facilities. The economic feasibility of AI therefore depends on whether operational improvements justify the costs of data infrastructure, computing resources, software development, maintenance, and technical personnel. Lightweight ML models, model compression, edge computing, and efficient training approaches may provide practical alternatives for applications with limited computational resources.

5.4. Cybersecurity, privacy, and data governance

Digitalized energy systems increasingly depend on interconnected sensors, smart meters, communication networks, cloud computing, and automated control systems. This connectivity creates potential cybersecurity vulnerabilities. Data manipulation, adversarial attacks, unauthorized access, and communication failures may compromise AI-based energy management. Data privacy is particularly important in residential energy management because smart-meter observations may reveal household occupancy and consumption behavior.
Federated learning offers a potential approach for collaborative model training without requiring all participating organizations to transfer their raw datasets to a central repository. Grataloup et al. (2024) identified its potential for addressing data-sharing limitations while emphasizing unresolved issues involving communication, privacy, fairness, and data heterogeneity. Nevertheless, federated learning should not be considered automatically secure. Secure aggregation, authentication, model-update protection, and appropriate governance remain necessary.

5.5. Environmental footprint of artificial intelligence

AI is frequently presented as an enabling technology for decarbonization, but its environmental footprint must also be considered. Training and operating computationally intensive models require electricity, data-center infrastructure, cooling systems, communication networks, and hardware manufacturing. The environmental impacts depend on computing efficiency, model architecture, electricity sources, hardware utilization, and equipment lifetimes. The IEA identifies the expanding electricity requirements associated with AI and data centers as an important consideration for future energy planning. This creates an important research question: under what conditions do the energy savings enabled by AI exceed the electricity and environmental burdens associated with its development and deployment? Answering this question requires lifecycle assessment and transparent reporting of computational energy consumption, rather than relying exclusively on model accuracy or computational speed.

5.6. Scalability, interoperability, and regulatory barriers

AI models developed for individual laboratories or simulation environments may encounter significant difficulties when transferred to operational electricity networks. Differences in equipment configurations, sensor

technologies, data formats, communication protocols, and regulatory requirements can limit interoperability. Furthermore, AI systems may require continuous recalibration as operating conditions change. Regulatory uncertainty concerning automated decision-making, liability, cybersecurity, and data ownership may also discourage deployment. Addressing these barriers requires coordination among energy companies, technology providers, regulators, researchers, and infrastructure operators.

6. Future research directions and emerging opportunities

The next phase of AI development in sustainable energy systems will require a transition from isolated predictive applications toward integrated, reliable, explainable, and sustainability-oriented intelligent infrastructure. Although current research demonstrates considerable potential, several technological and methodological developments are necessary to facilitate large-scale implementation.

6.1. Explainable and trustworthy artificial intelligence

Future research should prioritize explainable AI to improve transparency and confidence in intelligent energy-management systems. Advanced DL and RL models may achieve high predictive or operational performance, but their decisions can be difficult to interpret. This is particularly problematic when AI recommendations influence electricity dispatch, battery operation, grid stability, or critical infrastructure maintenance. SHAP, LIME, attention-based interpretation, and interpretable surrogate models can provide information about the variables influencing model predictions. Future investigations should move beyond explanation of individual predictions toward systematic evaluation of model reliability, uncertainty, robustness, and physical consistency. Trustworthy AI frameworks should also incorporate human oversight, cybersecurity safeguards, and clearly defined responsibilities for automated decisions.

6.2. Physics-informed and hybrid artificial intelligence

Integrating physical knowledge with data-driven learning represents an important opportunity for improving AI applications in energy systems. Conventional ML models may identify statistical relationships without necessarily respecting the underlying physical principles governing electricity generation, power flows, thermodynamics, or battery degradation. Physics-informed neural networks and hybrid physics–ML approaches can incorporate engineering equations and physical constraints into model development. For example, renewable energy forecasting models can integrate meteorological relationships, while battery-management models can incorporate electrochemical degradation principles. Hybrid AI approaches can also combine ML prediction, mathematical optimization, and engineering-based control. Future research should investigate whether these integrated approaches improve generalization, reduce training-data requirements, and enhance operational reliability compared with purely data-driven models.

6.3. Federated learning and distributed energy intelligence

The increasing decentralization of electricity infrastructure creates opportunities for distributed AI architectures. Federated learning enables multiple energy facilities, buildings, or organizations to contribute to collaborative model training without directly exchanging their raw datasets. This approach may be particularly relevant to smart-grid management, distributed renewable generation, and residential energy management. Future research

should investigate communication-efficient federated learning, model personalization, secure aggregation, and methods for addressing differences between participating datasets. Zheng et al. (2024) reviewed privacy-preserving federated learning for power-system services, while a separate review identified opportunities and implementation challenges for federated learning in renewable energy applications.

6.4. Digital twins and intelligent energy infrastructure

Digital twins are virtual representations of physical systems that can be updated using operational data. When combined with AI, they can provide platforms for simulation, monitoring, forecasting, and operational optimization.

In sustainable energy systems, digital twins may represent wind turbines, solar installations, battery systems, buildings, microgrids, and electricity networks. AI models can use digital-twin environments to evaluate alternative operating strategies and identify potential failures before implementing changes in physical infrastructure. For example, an intelligent digital twin of a microgrid could simulate alternative combinations of renewable generation, battery operation, and electricity demand under different weather conditions. Future studies should examine how digital twins can be integrated with physics-informed AI, predictive maintenance, RL, and real-time optimization. Importantly, digital-twin predictions should be continuously validated against actual operating conditions to prevent model drift and unrealistic simulation results.

6.5. Multi-agent reinforcement learning and decentralized energy management

Future electricity systems will increasingly involve interactions among multiple energy producers, storage operators, consumers, EVs, and distributed control systems. Multi-agent reinforcement learning offers an opportunity to coordinate these interconnected resources through decentralized or cooperative decision-making. For example, multiple buildings could independently optimize electricity consumption while coordinating with a community energy-management system. Similarly, distributed batteries and EV fleets could respond collectively to grid conditions without requiring a single centralized controller to process every operational decision. However, multi-agent approaches introduce challenges involving coordination, communication, reward design, convergence, and the prevention of conflicting actions. Future studies should investigate safe multi-agent learning and scalable coordination mechanisms under realistic electricity-market and network constraints.

6.6. Green AI and sustainability-oriented model development

The environmental footprint of AI should become an explicit component of sustainable energy research. Current AI studies frequently emphasize predictive accuracy and computational performance while providing limited information about electricity consumption, hardware requirements, or lifecycle impacts. Green AI research should prioritize computationally efficient models, renewable-powered computing, model compression, and energy-aware training strategies. Researchers should report relevant indicators, including training energy, inference energy, computational requirements, and the environmental characteristics of electricity supplies. Furthermore, lifecycle assessment can help determine whether AI-enabled improvements produce meaningful net environmental benefits. This research direction is especially important because the electricity demand associated with AI infrastructure is itself becoming a significant energy-sector consideration.

6.7. Integrated AI frameworks for net-zero energy systems

An important future direction is the development of integrated AI frameworks that connect renewable generation, electricity networks, storage, buildings, transportation, and industrial energy systems. Rather than developing separate forecasting and optimization tools, researchers should investigate interoperable platforms that coordinate these components through shared data infrastructures. Such platforms could combine ML and DL for renewable generation and demand forecasting; RL for adaptive control and operational decision-making; evolutionary algorithms for multiobjective energy optimization; digital twins for simulation and operational monitoring; federated learning for privacy-preserving collaboration; explainable AI for transparency and accountability; and lifecycle assessment for evaluating environmental performance. The objective should be to develop energy systems that are not only computationally intelligent but also economically viable, environmentally sustainable, resilient, and socially inclusive. Figure 3 presents an integrated research framework linking these emerging technologies with the future development of sustainable energy systems.

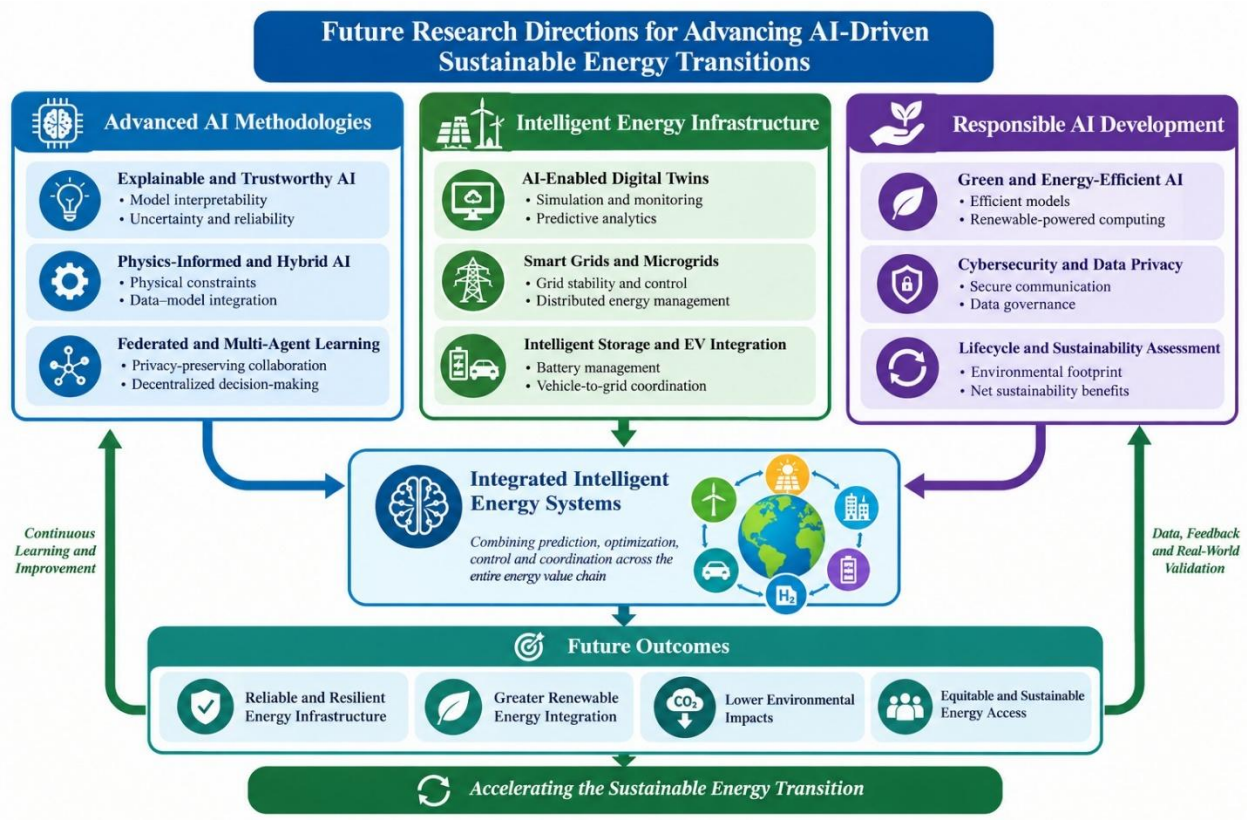

Figure 3. Research framework and future directions for advancing AI-driven sustainable energy transitions

7. Conclusions

Artificial intelligence represents an important technological enabler of the sustainable energy transition through its capabilities in prediction, optimization, adaptive control, and intelligent decision-making. This review demonstrates that ML, DL, RL, and intelligent optimization techniques can contribute to improving renewable energy forecasting, smart-grid management, energy storage, demand response, predictive maintenance, and integrated energy systems. ML provides flexible approaches for identifying patterns and predicting energy-system

behavior, while DL can represent complex temporal and spatial relationships. RL introduces adaptive decision-making capabilities, and intelligent optimization techniques can support resource allocation and operational planning. Their integration provides opportunities for developing more flexible, efficient, and renewable-compatible energy infrastructures.

However, the practical contribution of AI depends on addressing significant challenges associated with data quality, model interpretability, computational requirements, cybersecurity, scalability, and environmental impacts. The electricity consumption and infrastructure requirements of AI must also be considered when evaluating its overall sustainability contribution. Future research should prioritize explainable and physics-informed AI, federated learning, digital twins, multi-agent intelligent systems, and energy-efficient computational architectures. Equally important is the development of integrated assessment frameworks that evaluate not only algorithmic performance but also economic feasibility, lifecycle environmental impacts, system reliability, and social implications.

Ultimately, AI should be regarded not as an independent solution to energy-transition challenges but as an enabling component of broader technological, institutional, and policy transformations. Its successful deployment will depend on combining computational intelligence with sound engineering principles, responsible governance, and measurable sustainability objectives.

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