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Artificial intelligence and machine learning in optoelectronics and energy storage: From materials design to device applications

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ABSTRACT

Artificial intelligence and machine learning are reshaping materials science by accelerating the discovery, design, and optimization of materials for optoelectronic and energy storage applications. Optoelectronic and energy storage devices, including photovoltaics, light-emitting diodes, batteries, and supercapacitors, are significantly affected by increasing demands for performance, multifunctionality, and sustainability. Conventional trial-and-error methods often fail to address these challenges, making data-driven approaches critical for driving innovation. This review presents the fundamental principles of artificial intelligence and machine learning in materials science, including core algorithms, data acquisition and preprocessing, feature engineering, and interpretable modeling strategies. Recent advances in artificial intelligence-driven optoelectronic devices, such as photovoltaics, light-emitting devices, and photodetectors, are discussed alongside developments in energy storage systems, including batteries, supercapacitors, and hybrid devices. Emphasis is placed on data-driven discovery of electrodes and electrolytes, as well as on predictive modeling of charge–discharge behavior and degradation mechanisms. The review further highlights integrated and cross-cutting applications, including coupled optoelectronic–energy storage systems, multifunctional device design, inverse materials discovery, and artificial intelligence-enhanced multiphysics simulations, with particular attention to emerging hybrid architectures. Key challenges are critically analyzed, including data scarcity and bias, limited generalization across materials systems, interpretability–accuracy trade-offs, and the gap between computational predictions and experimental validation. Practical strategies are proposed to address these limitations and improve model reliability. Finally, future perspectives are outlined, focusing on autonomous experimentation, quantum computing-enhanced artificial intelligence, sustainable approaches, and industrial translation. This review provides a cohesive framework linking materials design to device applications, offering insights for the development of next-generation intelligent materials and energy technologies.

1. Introduction

The global energy issue has worsened in recent years, driven by increased industrialization and urbanization, as well as the rising need for sustainable and reliable power supplies. The environmental effects of fossil fuels and the pressing need to address climate change have driven research toward sustainable energy systems and advanced energy storage solutions [1]. Photovoltaics and light-emitting diodes (LEDs) are key

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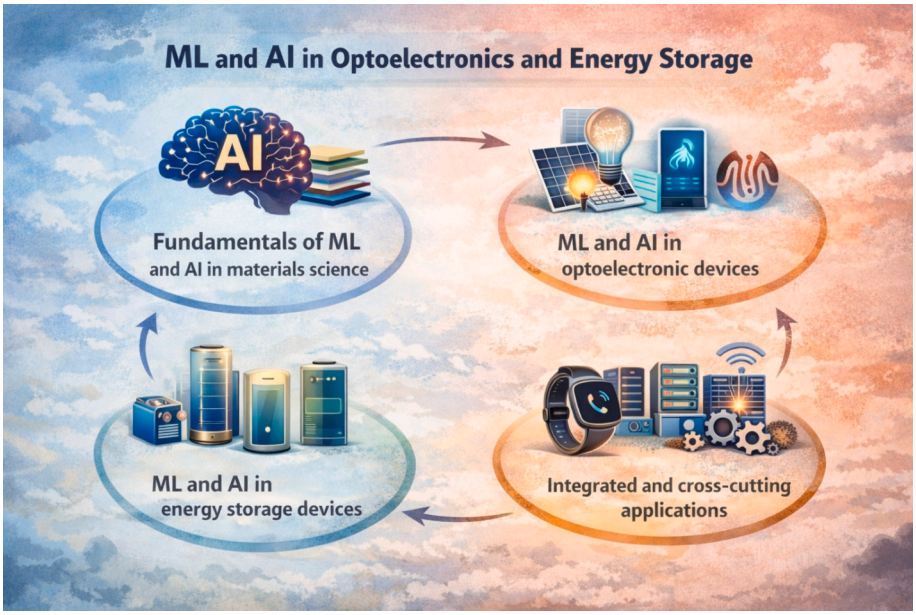
components in energy harvesting and conversion, while batteries and supercapacitors are required for efficient storage and usage. Despite significant advancements over the past decades, these technologies continue to face key limitations in performance, sustainability, scalability, and affordability [2]. Traditional trial-and-error approaches to materials discovery and device optimization frequently lack the urgency and performance required to address contemporary energy challenges [3]. Artificial intelligence (AI) and machine learning (ML) have become significant tools for advancing the discovery and development of advanced materials and devices. AI/ML effectively extracts patterns from large, complex datasets, revealing hidden relationships and trends that conventional analysis often overlooks. These tools predict material properties, screen extensive chemical and structural spaces, and facilitate experimental design, significantly reducing the time and resources required for trial-and-error experimentation [4]. AI/ML facilitates a transition to a systematic, data-driven methodology in materials science, enabling hypotheses to be tested in silico before laboratory validation. This accelerates innovation and facilitates the discovery of new classes of materials and device structures that may otherwise remain unexplored. AI/ML can enhance performance, increase stability, and enable multifunctional structures in optoelectronic and energy storage technologies, underscoring their significant role in addressing contemporary energy and sustainability challenges [5].

Although significant progress has been made in AI and ML for materials and device research, most studies conducted over the last five years or more remain largely confined to specific domains. Research has primarily focused on optoelectronic devices, such as photovoltaics and LEDs, or energy storage technologies, such as batteries and supercapacitors. There is a notable limitation of studies investigating integrated, multipurpose devices that combine energy harvesting and storage [6]. The limited cross-disciplinary integration limits the ability to fully leverage the predictive and advanced features of AI/ML across interconnected devices, which are becoming increasingly significant for self-powered sensors, wearable electronics, and photo-rechargeable batteries. Moreover, substantial methodological and infrastructural challenges persist. Numerous datasets are characterized by small size, fragmentation, or bias, which impedes the advancement of generalizable models. The lack of standardized criteria for evaluating algorithmic performance complicates comparisons across studies. Complex models, including deep neural networks (DNNs) and generative structures, often exhibit limited interpretability, which diminishes their ability to inform experimental design [7]. A persistent gap exists between computational predictions and experimental validation. Although AI and ML can identify promising material candidates or device designs, translating these predictions into reproducible experimental results remains a challenge. The identified limitations hinder the adoption of AI-driven perspectives in practical device growth, underscoring the necessity for integrated, standardized, and interpretable AI/ML systems to expedite the advancement of multifunctional energy technologies [8].

This review examines the existing gaps by offering a comprehensive overview of the impact of AI/ML on optoelectronic and energy storage systems within a cohesive framework. In contrast to previous reviews that typically focus on a specific device category or algorithms in isolation, this review highlights comprehensive strategies that include inverse design, generative models, transfer learning, and the integration of computational and experimental approaches. This review emphasizes emerging themes such as multifunctional device architectures, autonomous laboratories, and green AI approaches, which have not been thoroughly examined in existing literature. This review seeks to integrate advancements across various domains, providing a critical evaluation of existing challenges and a prospective outlook on the role of AI and ML in enhancing the discovery and implementation of next-generation energy technologies. The main features of this review are given in Scheme 1.

2. Fundamentals of ML and AI in materials science

Materials science has been revolutionized by the addition of AI and ML, which have changed the way researchers identify, develop, and enhance materials. Historically, materials development has relied on intuition-based experimentation and trial-and-error synthesis, often time-consuming and resource-intensive [9]. Conversely, ML and AI offer data-driven approaches that can reveal complex structures, forecast material properties, and accelerate discovery. This section defines the fundamental principles of ML and AI as they pertain to materials research. It starts with a description of typical algorithms and learning paradigms, then moves on to data gathering and preprocessing, which are essential stages for assuring model precision and reliability. This section analyzes feature engineering and descriptor design, which serve as intermediaries between raw material data and meaningful machine representations. It ultimately discusses model interpretability and explainability, highlighting the importance of transparent, reliable AI



Scheme 1. Graphical illustrations of the main features of AL/ML are addressed in this review.

systems for improving fundamental understanding and guiding experimental validation.

2.1. Core algorithms and approaches

ML and AI serve as revolutionary tools in materials science, providing data-driven approaches to elucidate complicated relationships among composition, structure, and performance. These approaches overcome the limitations of conventional trial-and-error investigation by facilitating statistical modeling, performance enhancement, and automated exploration [10]. ML algorithms are classified into four main categories: supervised, unsupervised, reinforcement, and deep learning paradigms. Supervised learning techniques, including regression and classification models, are employed to predict material properties or classify materials utilizing established datasets [11]. Unsupervised learning identifies latent structures and

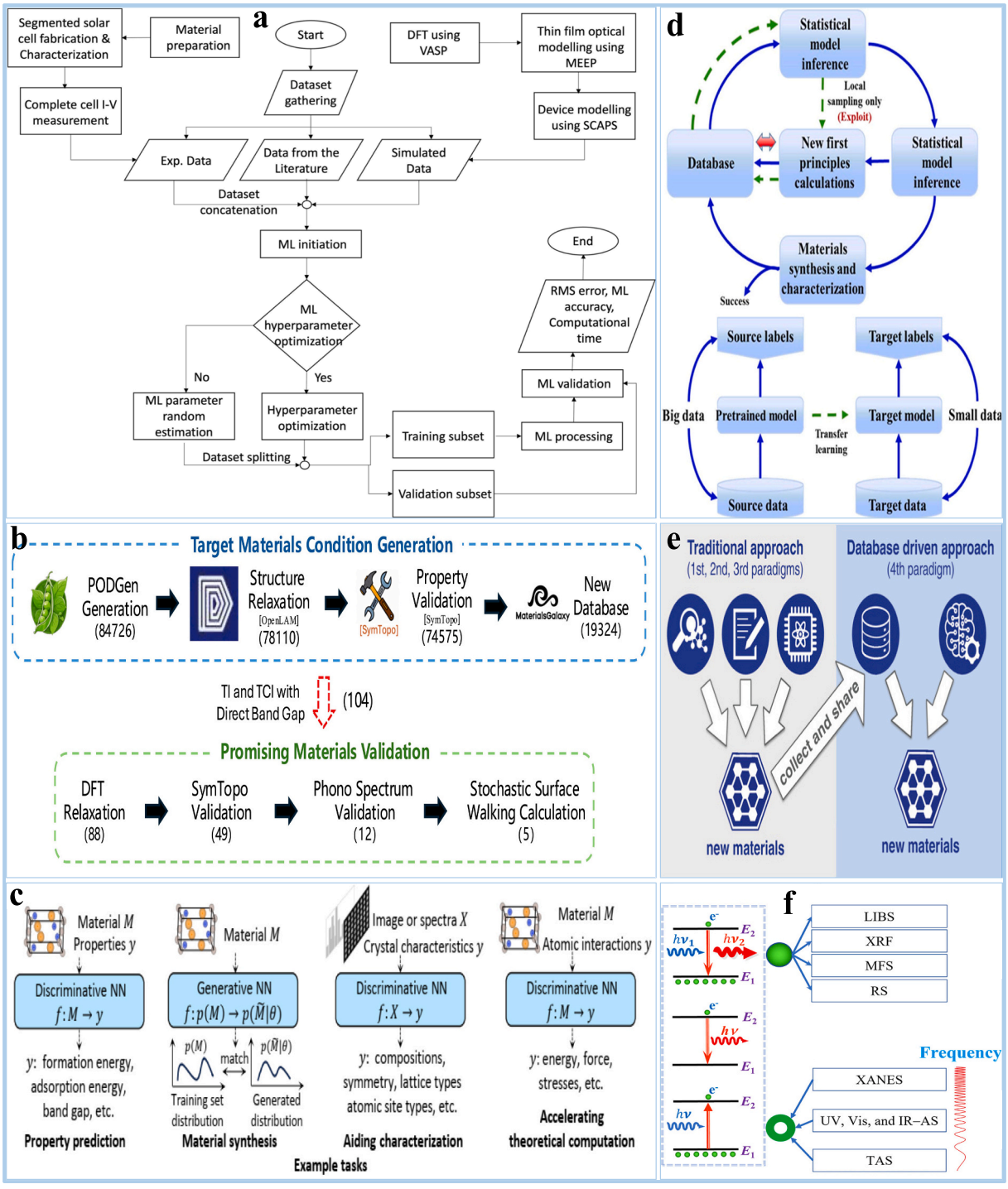


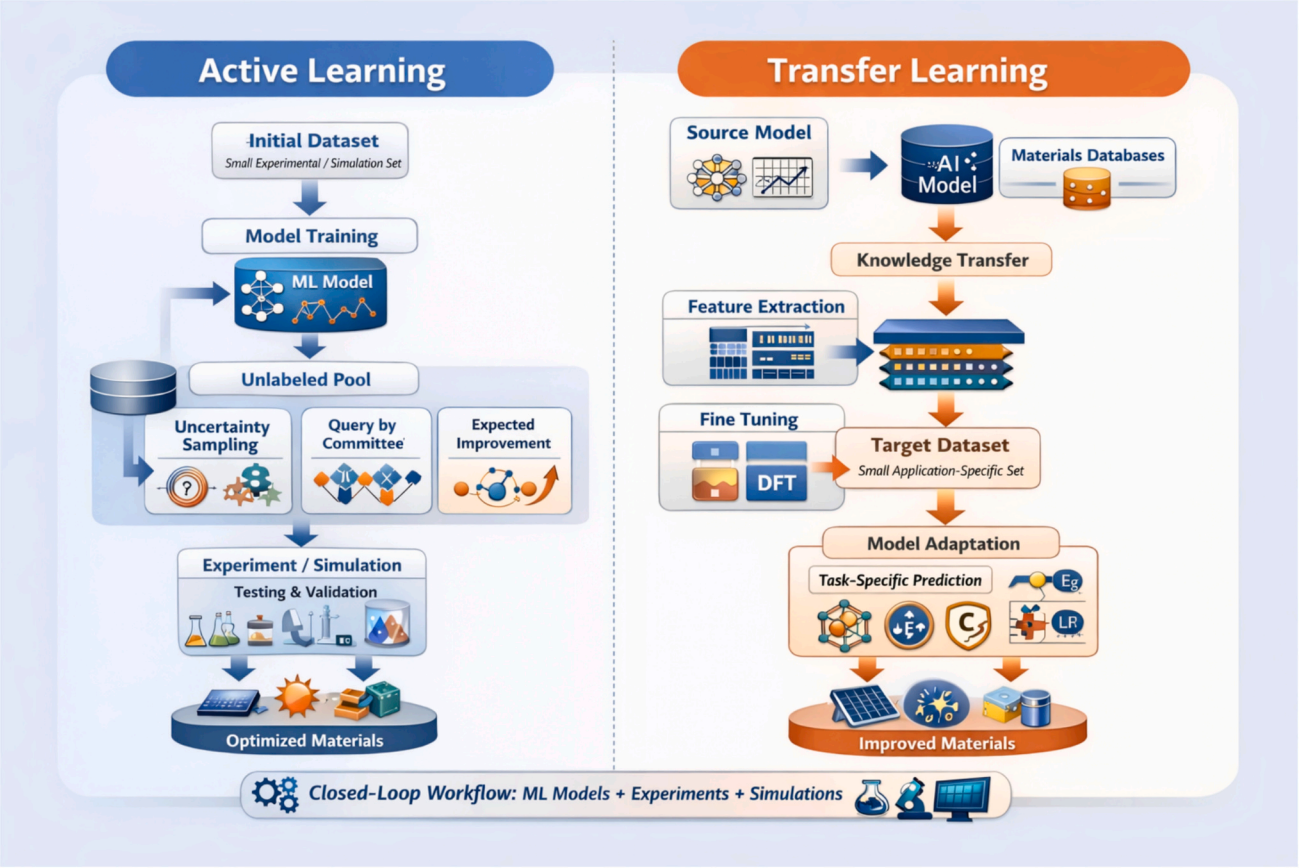
Fig. 1. (a) Flowchart of the entire process [15]. Copyright © 2024, Springer. (b) Graphic representation of the study process: a conditional generative structure for crystal formation, succeeded by structural enhancement, screening, and first-principles validation [16]. Copyright © 2025, Nature. (c) Analysis of deep learning applications in crystalline materials [17]. Copyright © 2026, ACM.org. (d) Schematic overview of active and transfer learning [21]. Copyright © 2023, Nature. (e) Materials discovery schematic revolutionary [22]. Copyright © 2019, John Wiley and Sons. (f) Schematic diagram of spectral technology principle [23]. Copyright © 2025, Elsevier.

categorizes data based on shared features, without predefined labels [12]. Reinforcement learning and DNNs have recently attracted attention for their ability to handle complex, nonlinear, and high-dimensional datasets, making them particularly useful in materials design and process optimization [13]. Grasping these algorithmic foundations enables researchers to choose appropriate models, balance accuracy with interpretability, and tailor computational techniques to experimental workflows, thereby expediting advancement in materials discovery and device engineering [14]. For example, Omar et al. [15] conducted a detailed assessment of ML algorithms for photovoltaics, focusing on their precision and computational costs across datasets varying in generation, size, and complexity. Their research thoroughly examined five different ML algorithms, ranging from basic linear and polynomial regression to more advanced methods such as random forest, neural network, and a hybrid model that integrates the latter two. Their approach involved testing each algorithm with and without hyperparameter optimization, enabling quantification of the trade-off between the high computational cost of modification and the resulting gains in model precision. They employed five distinct datasets to enhance the reliability of thier findings, encompassing a diverse array of photovoltaic technologies, such as standard silicon p–n-junction devices, dye-sensitized solar cells (DSSC), perovskite solar cells (PSC), and advanced perovskite-on-silicon tandem designs. This method enabled the authors to assess ML efficiency in relation to essential dataset attributes, including size (number of data points), attributes (number of inputs and outputs), and conduct (the intrinsic properties of the solar device) (Fig. 1a). The results showed the superior performance of the Random Forest algorithm, achieving exceptional precision with a root-mean-square error (RMSE) of approximately 9.21×10^{-07} across diverse datasets. Their study further conducted a detailed analysis of hyperparameter optimization's effects, demonstrating that its effect is significantly dependent on the model's complexity. The neural network with the highest parameter count showed the greatest improvement in accuracy after optimization, underscoring that, despite being computationally intensive, such tuning is essential for complex models to realize their full predictive potential. Similarly, Ye et al. [16] presented a conditional generative model, PODGen, to enhance materials discovery by integrating generative AI with property-prediction algorithms. Conventional generative methods, including diffusion and autoregressive models, show promise for material exploration but are ineffective for targeted design. PODGen overcomes this limitation by combining a general generative model with multiple property predictors, enabling more effective, high-throughput conditional formation of crystallized materials. Employing this structure, the authors concentrated on identifying novel topological insulators (TIs). The results indicated that PODGen achieved a 5.3-fold increase in success rate compared to unconstrained generation techniques and demonstrated a distinct efficiency in generating gapped TIs, which are rarely produced by general approaches. The model produced numerous candidate materials, which were later confirmed through first-principles calculations of the most intriguing structure. Newly discovered and potentially synthesizable topological insulators include CsHgSb, $NaLaB_{12}$, $Bi_4Sb_2Se_3$, Be_3Ta_2Si, and Be_2W (Fig. 1b). Their study illustrates the significant improvements in performance and accuracy of targeted materials discovery achieved through conditional generative modeling. Furthermore, Wang et al. [17] investigated the use of AI and deep learning to advance the discovery of crystalline materials. Crystalline materials possess periodic atomic structure and exhibit a range of functional properties, making them essential in fields like electronics and energy. However, conventional discovery methods tend to be inefficient and expensive. They investigated data-driven methods to address these limitations, utilizing the increasing accessibility of materials data. They analyzed various data representations, such as geometric graphs, string notations, images, and spectra, and employed deep learning models, such as graph neural network, language models, and convolutional neural network, to accurately capture and predict intricate atomic interactions in crystal structures. These models have been shown to facilitate essential tasks, including the prediction of physicochemical properties, material synthesis, characterization, and the rapidity of theoretical computations (Fig. 1c). Their research emphasized frequently utilized datasets, benchmarks, and software, while pinpointing challenges that need to be overcome to fully connect the properties of deep learning for effective and precise AI-assisted crystalline materials discovery.

2.2. Data acquisition and preprocessing

Data constitute the basis of all ML and AI models, with the quality of the input data directly influencing the reliability of predictions. In materials science, data are sourced from various origins, including experimental databases like Materials Project, AFLOW, and NOMAD, computational simulations such as DFT calculations, and high-throughput synthetic or characterization studies [18]. These datasets often differ in format, scale, and reliability, requiring careful preprocessing before modeling. Preprocessing encompasses critical steps, including data cleaning to address missing or inconsistent entries, normalization for comparability, feature scaling to reduce the influence of high-magnitude variables, and outlier detection to remove unrealistic values [19]. In materials data, it is essential to maintain physical meaning during conversion, as inadequate preprocessing can distort fundamental relationships. Advanced methodologies, such as automated data curation and data augmentation through generative models, are currently being implemented to enlarge constrained datasets and improve model robustness [20]. Ultimately, thorough data collection and preprocessing ensure that ML predictions remain scientifically valid and physically significant. For example, Xu et al. [21] investigated strategies for applying ML in materials science under conditions of limited data availability, with particular emphasis on data acquisition and preprocessing methods. Their study focused on addressing small-data challenges by extracting information from published literature, developing dedicated materials databases, performing high-throughput computational and experimental studies, and designing algorithms tailored to handle small or imbalanced datasets. They employed ML methods, including active learning and transfer learning, to enhance model performance. They investigated methods to address small-data challenges in materials science by integrating active and transfer learning techniques. Active learning involves iteratively selecting the most informative samples from a large pool of unlabeled data, which are then labeled and added to the training set. The training, scoring, labeling, and retraining processes continue until the model achieves adequate precision. This method in materials design enables ML models to suggest candidate materials for experimental or computational validation, which are then incorporated back into the training set, facilitating ongoing enhancement of both the data and the model. They further examined transfer learning to utilize knowledge from extensive, well-defined datasets in a source domain to enhance predictions in target domains with constrained data availability. A pre-trained model is initially developed using extensive source-domain data and subsequently refined with limited target-domain datasets to improve predictive accuracy. Although alternative methods, such as relation-based or sample-weighted transfer, are available, model-based transfer is predominantly used in materials research (Fig. 1d). Their work offers practical methodologies for effectively applying ML in materials research for data acquisition and preprocessing.

To further provide practical guidance for materials scientists, the implementation workflows of active learning and transfer learning are illustrated in Scheme 2. The figure outlines how active learning iteratively selects the most informative samples using strategies such as uncertainty sampling and model disagreement, followed by experimental or computational validation and continuous model updating. In parallel, the transfer learning workflow demonstrates how knowledge from large-scale source datasets can be adapted to target tasks with limited data through fine-tuning and feature reuse. These integrated workflows



Scheme 2. Workflow illustration of active learning and transfer learning strategies for efficient data-driven materials design in optoelectronic and energy storage applications.

establish a closed-loop structure that connects machine learning, simulations, and experiments, thereby enabling efficient materials discovery and optimization in optoelectronic and energy storage systems. Similarly, Himanen et al. [22] conducted a detailed investigation into enhancing data-driven materials science by integrating extensive materials datasets with ML and high-throughput computational methods to expedite materials discovery and development. They highlighted the importance of incorporating diverse data sources, including experimental evaluations and theoretical simulations, to uncover complex structure–property–performance relationships that traditional methods often fail to access. They proposed a structure that enhances data reliability, standardization, and interoperability across diverse databases, thus guaranteeing a uniform and adaptable information flow within the materials research community. The research highlighted the importance of open-access infrastructure and effective data management practices for enabling automated data analysis and predictive modeling. Through the application of these principles, they demonstrated that data-driven workflows can effectively identify promising material candidates, lower discovery costs, and inform experimental validation (Fig. 1e). Their work demonstrated the revolutionary potential of AI and big data analytics in advancing materials design and innovation. Furthermore, Yan et al. [23] designed and refined a comprehensive structure for spectral data preprocessing to enhance the performance and precision of ML-based quantitative material evaluation. The authors systematically investigated techniques to reduce variations in spectroscopic data caused by noise, instrumental drift, and environmental interference during data acquisition and preprocessing. The workflow included essential methods such as cosmic-ray and baseline correction, scattering and normalization corrections, filtering and smoothing, and the application of spectral derivatives to improve signal clarity and extract significant features. To enhance data quality, adaptive, physics-constrained preprocessing approaches were introduced that dynamically adjust to changes in sample conditions and measurement environments. The advanced methodologies preserved the physical integrity of spectral knowledge, enhanced feature consistency, and minimized bias in ML training datasets. The study showed that well-structured preprocessing pipelines improved model reliability and generalization, leading to a notable rise in predictive efficiency in quantitative analysis (Fig. 1f). Their research highlighted the essential importance of intelligent data acquisition and preprocessing in facilitating precise, reproducible, and high-sensitivity spectral analysis for applications in materials science.

2.3. *Feature engineering and descriptors*

Feature engineering is an essential process that converts unprocessed data into organized, machine-readable formats that precisely represent the fundamental physics and chemistry of a system. In materials science, these features, referred to as descriptors, provide quantitative descriptions of atomic, electronic, structural, and thermodynamic properties [24]. Well-structured descriptors allow ML models to discern significant relationships between a material's composition and its observable properties. Common descriptor types encompass atomic-level properties (e.g., atomic radius, electronegativity, and valence electron counting), structural descriptions (e.g., coordination number, bond angles, and lattice constants), and electronic descriptions (e.g., bandgap, Fermi energy, and density of states) [25]. In device-related projects, factors such as charge transfer, dielectric constant, and surface energetics are utilized. The performance of an ML model is significantly affected by the relevance and diversity of its descriptors.

Advanced descriptor generation techniques, such as graph-based and deep learning approaches, have improved predictive accuracy by effectively capturing both local and global structural information [26]. Successful feature engineering serves as a connection between domain knowledge and computational intelligence, facilitating both foundational understanding and focused material design. For example, Kalidindi et al. [27] examined the advancement of AI-based Materials Knowledge Systems (AI-MKS) by emphasizing feature engineering methods that encapsulate the internal structure of materials via lower-dimensional descriptors. The descriptors were developed to capture the essential process-structural-property relationships across multiple length scales, providing a basis for effective ML-based surrogate models. The structure integrates AI and ML tools with theoretical and physics-based simulations, facilitating a systematic and data-driven method for estimating and enhancing material behavior while minimizing computational costs (Fig. 2a). They showed that a large MKS should serve as an organized repository of PSP linkages, wherein uncertainties can be assessed, and the connections between preparation, structure, and properties are distinctly defined. They identified a significant challenge: the lack of standardized taxonomies, variables, and datasets required for the development of such structures. To fill this gap, the authors emphasized the importance of integrated information infrastructures, such as the materials data curation system (MDCS) developed at NIST, which enables consistent labeling, organization, and sharing of materials data. Collectively, these initiatives establish a scalable, interoperable structure that accelerates materials discovery and innovation. Similarly, Anand et al. [28] examined topological feature engineering as a method to enhance ML-based development of zinc halide perovskite materials for photovoltaic usages. It was revealed that geometry and topology serve as the structural framework for physical and materials simulations, highlighting the need for more fundamental and generic descriptors beyond conventional parameters such as atomic and ionic radii and the tolerance factor. To overcome this limitation, a multiscale simplicial complex structure was developed utilizing persistent functions (PFs), which effectively captures both geometric shape and topological connectivity in organic–inorganic halide perovskites (OIHPs). This method offers enhanced abstraction and structural accuracy, enabling ML models to better capture intricate atomic relationships. Their PF-based models exhibited markedly superior predictive accuracy and transferability compared to traditional descriptor-based methods, achieving performance levels comparable to those of advanced deep learning models. Combining geometrical and topological properties as molecular attributes revealed an additional link between structure and properties, such as bandgap dynamics, which improved the accuracy of data-driven estimations (Fig. 2b). Their study demonstrates that mathematically rigorous, topology-informed feature engineering can enhance the discovery of perovskite materials and provide a structure for wider AI-assisted materials development. Furthermore, Dai et al. [29] investigated the application of ML and feature engineering to predict phase growth in high-entropy alloys, addressing the persistent challenge of identifying stable single-phase solid-solution structures. Traditional methods, including trial-and-error and thermodynamic models, are often time-intensive or constrained by the precision of their descriptors, leading to variable predictions. To address these limitations, the researchers implemented an advanced feature engineering method that increased descriptor dimensionality via nonlinear combinations, enabling ML models to more effectively capture the intricate interactions that influence HEA behavior (Fig. 2c). This approach markedly enhanced prediction accuracy relative to conventional techniques. Their study extended beyond high-entropy alloys, demonstrating the broader applicability of this approach to materials structures with small or incomplete datasets, underscoring its potential as a platform for data-efficient materials development. In addition, to clearly elucidate the differences between conventional ML methods and those tailored for materials science, a schematic comparison is provided in Scheme 3. In contrast to conventional ML pipelines that depend on extensive datasets and generic properties, materials-informed ML methods integrate domain-specific information, physics-informed preprocessing, and tailored descriptor generation. Supplementary measures, including domain-constrained model training, interpretability assessments, and experimental validation, guarantee that predictions comply to essential physical principles and can be empirically confirmed. This visual summary underscores the essential role of feature engineering and descriptors in connecting computational intelligence with materials science, illustrating how incorporating domain knowledge converts a generic predictive pipeline into a physics-informed, experimentally validated structure suitable for materials discovery and device optimization.

2.4. Interpretable and explainable models

Interpretability and explainability have become essential for maintaining transparency and scientific credibility as ML and AI models become more complex. High-performance models such as DNNs often operate as “black boxes,” offering little transparency into the rationale behind their predictions [30]. In materials research, comprehending the structure–property relationship is important. Interpretable AI not only provides accurate predictions but also helps identify governing processes and supports experimental validation [31]. Explainable AI (XAI) techniques, including feature importance mapping, shapley additive explanations (SHAP) values, local interpretable model-agnostic explanations (LIME), and surrogate modeling, elucidate the input properties that significantly affect predictions [32]. These techniques improve confidence in computational results and help researchers refine hypotheses or discover new materials. Interpretable models facilitate responsible AI applications by minimizing biases and enhancing reproducibility in scientific processes. Explainable ML integrates predictive properties with transparency, enhancing the relationship between data-driven modeling and the foundational concepts of materials science [33]. For example, Kailkhura et al. [34] built a robust and interpretable ML system designed to address ongoing challenges in materials exploration, particularly in the context of deficient, sparse, or underrepresented datasets. The authors identified common pitfalls of traditional ML models, noting that standard performance metrics often fail to yield meaningful evaluations in the presence of data imbalance and that model confidence scores may be misleading. Furthermore, efforts to improve interpretability through simplified models often resulted in reduced predictive accuracy, highlighting a significant trade-off between reliability and interpretability in materials information technology (Fig. 2d). The authors suggested a general-purpose ensemble-based ML system to enhance the reliability and interpretability of projections. This system integrates several simple models into an ensemble that delivers reliable, precise predictions while ensuring transparency. It also integrates transfer learning to leverage correlations across various material properties, facilitating learning from limited or unbalanced datasets. The research introduced novel evaluation metrics and trust scores to enhance the quantification of prediction confidence, along with a rationale generator that offers explanations for the outcomes at both the model and decision levels. Similarly, Oviedo et al. [35] investigated the function of interpretable and explainable ML in the fields of materials science and chemical science. The authors highlighted that, in addition to predictive accuracy, ML models should elucidate their internal mechanisms to foster trust, identify limitations, and expose unforeseen correlations that may facilitate scientific advancement. The research delineated core principles of interpretability and explainability, examined the trade-offs between explainability, completeness, and scientific validity, and offered methodologies for developing interpretable models. Their work demonstrated applications in first-principles calculations, materials evaluation, and experimental research, emphasizing the role of explainable models in guiding the invention of materials and their incorporation into complicated structures. Their study also

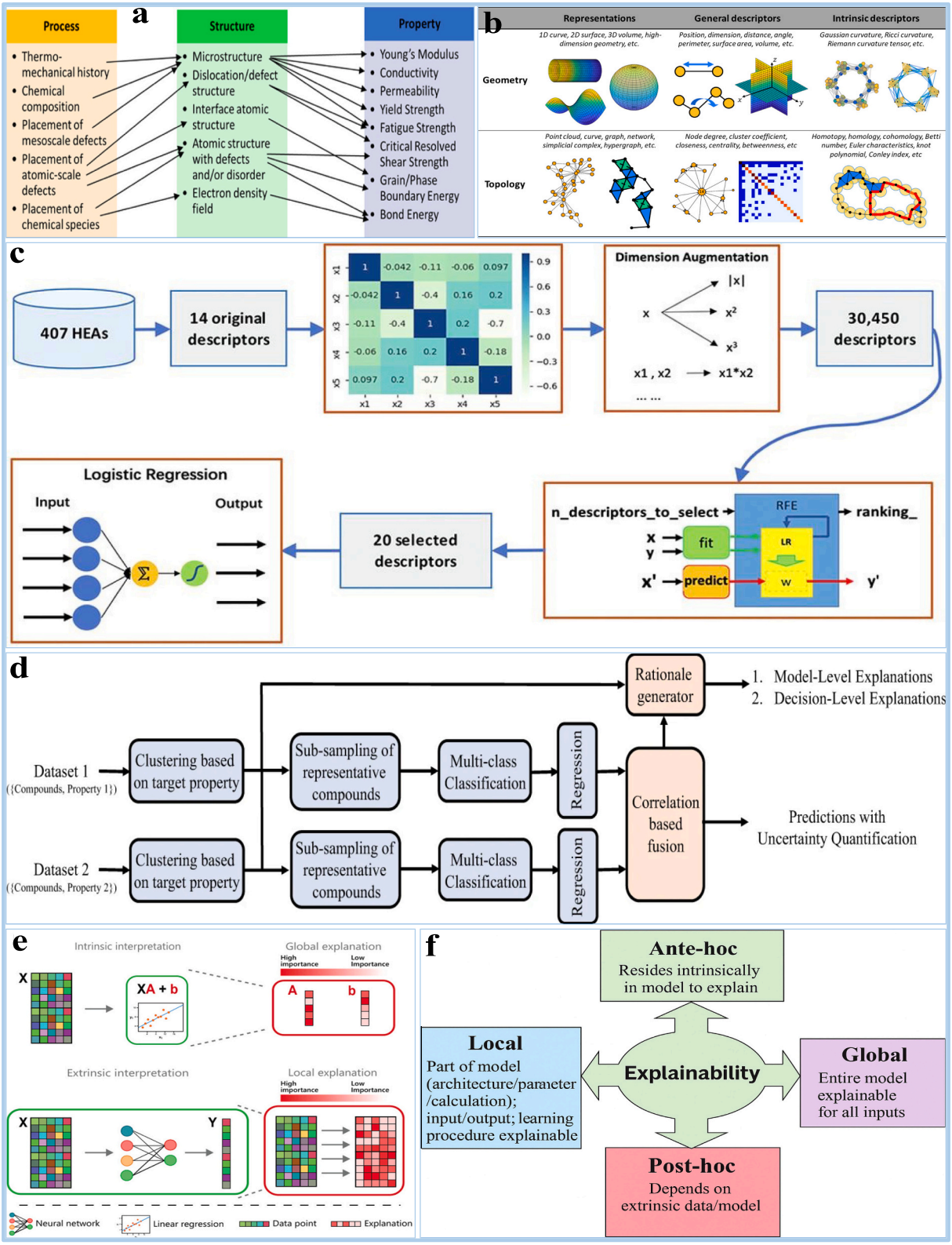
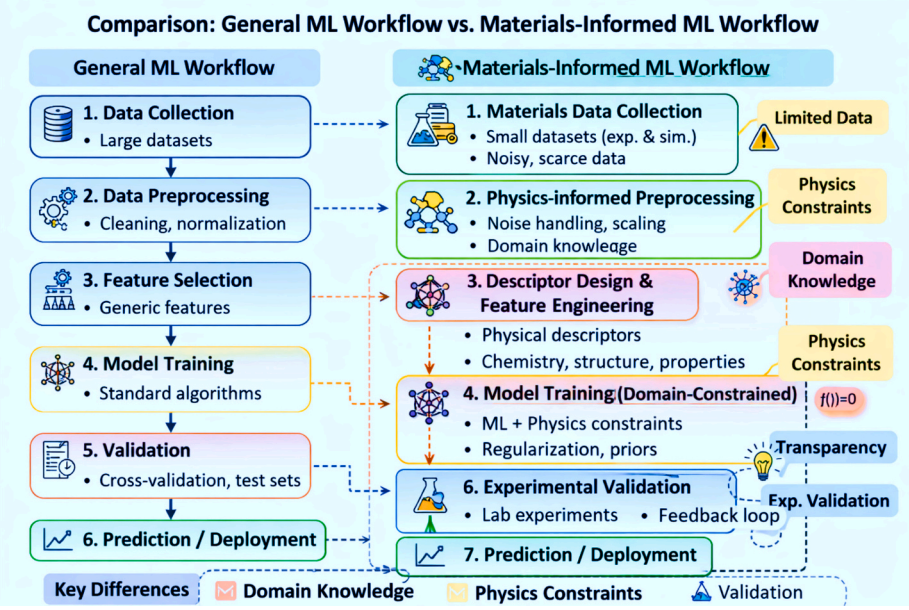


Fig. 2. (a) Graphical illustrations of the many variables used in the hierarchical PSP links' formulation [27]. Copyright © 2020, AIP Publishing. (b) Graphical illustrations of geometrical and topological structures, as well as generic and intrinsic descriptors [28]. Copyright © 2022, Nature. (c) A visualization of the original 14 descriptors' Pearson correlation coefficient matrices and the overall formation process [29]. Copyright © 2020, Elsevier. (d) A depiction of the proposed ML pipeline for predicting material properties [34]. Copyright © 2019, Nature. (e) A graphical representation of local and global definitions, as well as intrinsic and extrinsic interpretability [35]. Copyright © 2022, American Chemical Society. (f) Various dimensions and facets of explainability [36]. Copyright © 2022, Nature.



Scheme 3. Comparison of a general ML workflow (left) and a materials-informed ML workflow (right).

examined challenges, including the avoidance of overgeneralization and incorrect causal inference, as well as the significance of integrating uncertainty estimates (Fig. 2e). Their study illustrated that interpretability can be successfully integrated into ML workflows through practical examples and accessible tools, thereby improving reliability and scientific insight in materials research. Furthermore, Zhong et al. [36] investigated the use of XAI in materials science to tackle the issue that highly accurate ML models, including DNNs, frequently lack interpretability. The integration of explainability into ML workflows is vital for improving understanding, trust, and practical utility in materials research. They elucidated essential theories to enhance the accessibility of XAI for materials researchers. A model is deemed transparent when all its components are easily comprehensible, and it is intrinsically explainable if aspects of the model, such as functional forms or parameters, are based on physical principles. For non-transparent models, explanations can be offered extrinsically via simplification, supporting data, or proxy models that replicate the original black box. These explanations may concentrate on particular model components, inputs, or the learning process instead of the complete model. They noted that descriptions of transparency and explainability differ in the literature; however, for clarity, they do not differentiate between interpretability and explainability, thereby enhancing accessibility for practitioners in materials science (Fig. 2f). Their work establishes a structured system for integrating XAI into materials studies, allowing researchers to extract insights from complicated models while ensuring reliability and interpretability.

3. ML and AI in optoelectronic devices

The integration of ML and AI into optoelectronic research has facilitated significant advancements in the development, improvement, and exploration of next-generation technologies. Traditional experimental methods, though essential, often face constraints on time, cost, and the complexity of interactions between materials and devices [37]. AI and ML data-driven approaches that can effectively traverse complex landscapes, forecast efficiency metrics, and reveal correlations that traditional approaches may neglect. In optoelectronics, computational tools have shown significant potential for accelerating the development of high-performance photovoltaic structures, next-generation LEDs, sophisticated photodetectors, and novel flexible or neuromorphic photonic platforms [38]. This section examines the application of ML and AI in various optoelectronic fields, emphasizing significant advancements and persistent challenges.

3.1. Photovoltaics

Photovoltaic technologies, such as organic, perovskite, quantum dots (QDs), and tandem solar cells, have progressed significantly; however, issues related to performance, stability, and adaptability remain unresolved. The interactions among material composition, crystal structure, interactions, and device structure influence optimization [39,40]. ML and AI offer a data-centric methodology to enhance materials discovery and device design. AI and ML models efficiently evaluate extensive libraries of absorber materials, forecasting bandgap, carrier accessibility, defect tolerance, and stability, thereby helping researchers focus on the most promising candidates [41]. In addition to material choice, these tools improve device designs by analyzing layer thicknesses, junctions, and compositional gradients, thereby enhancing performance and operational lifetime. In tandem and multi-junction cells, AI identifies synergistic layer combinations, whereas in QDs and hybrid structures, ML captures complex, non-linear interactions among synthesis conditions and device performance [42]. These strategies facilitate accurate, expedited growth in photovoltaic systems, aiding the formulation of effective, reliable, and economically feasible solar energy technologies. For example, Nguyen et al. [43] utilized ML to forecast the yearly energy output of 4-terminal perovskite/silicon tandem photovoltaic (PV) cells intended for building-integrated applications (BIPV). An artificial neural network (ANN) model was designed utilizing inputs including solar irradiance, visible light angle, module temperature, perovskite absorber thickness, and bandgap. The ANN structure was improved using a surrogate algorithm, resulting in a three-hidden-layer architecture that demonstrated superior predictive efficiency (MSE = 0.02283, R = 0.99999, Willmott's index = 0.99999), while also assessing the relative significance of each input variable. The improved model forecasted the highest annual energy outputs at a perovskite bandgap of 1.71 eV, varying from 97.6 to 297.73 kWh/m^2 for rooftop and façade orientations, illustrating the performance of ML in estimating BIPV efficiency without the need for extensive experimentation (Fig. 3a). Their study indicates that while multiple ML models, including fuzzy logic, support vector regression, Gaussian process regression, and random forests, have been utilized for photovoltaic performance estimation, ANN demonstrate enhanced accuracy and simplicity. Improving the number of

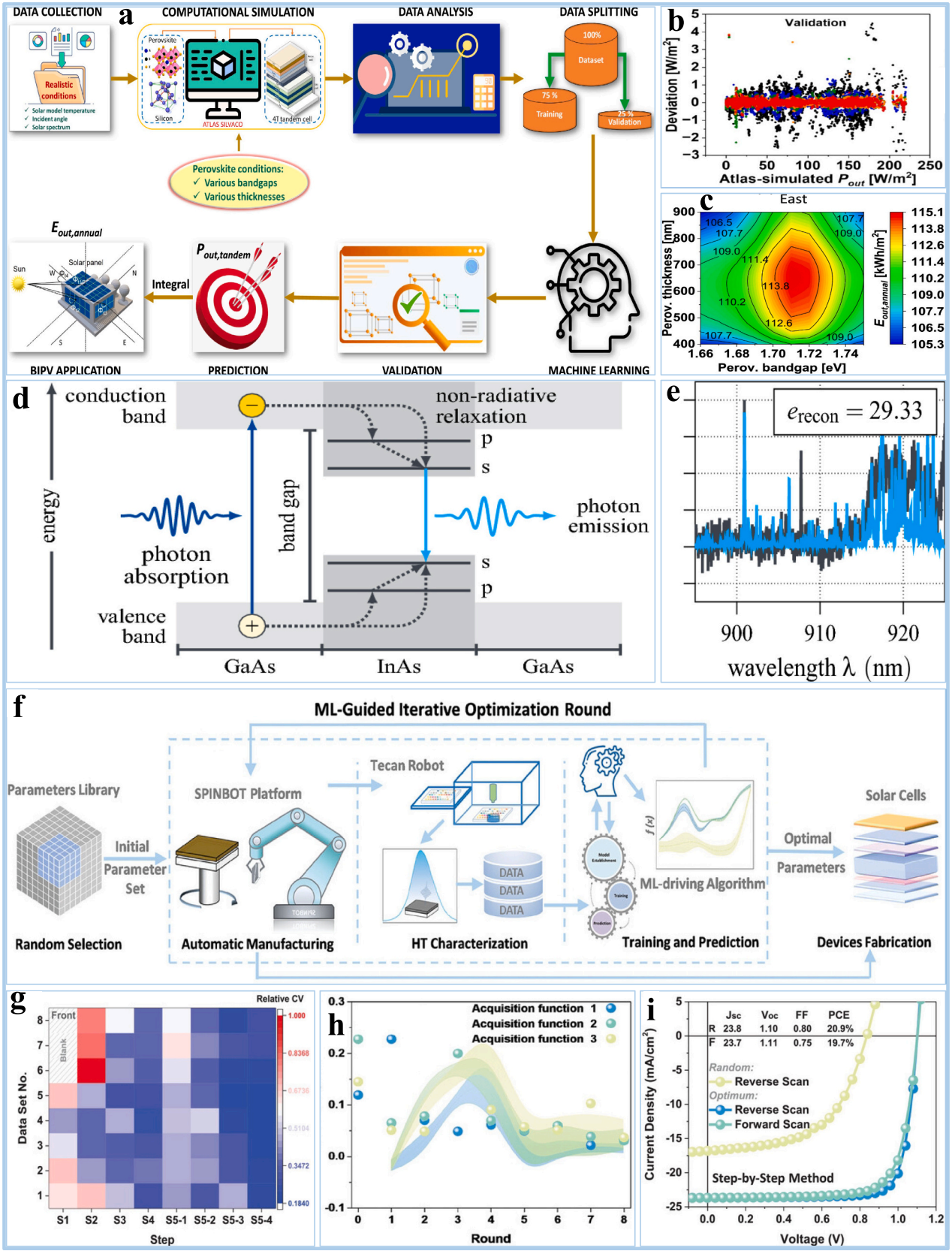


Fig. 3. (a) The fundamental structure of the intelligent structure for forecasting the tandem $E_{out,annual}$ for the BIPV; (b) The deviation values between the target and predicted P_{out} values for five predictive ANNs; (c) The corresponding contour plots and color mapping spectra [43]. Copyright © 2023, Elsevier. (d) A graphic representation of semiconductor QDs' fluorescent single photon emission; (e) Autoencoder reconstruction of three model QD emission [44]. Copyright © 2024, Nature. (f) Closed-loop tuning for film uniformity and quality guided by machine learning; (g) Color maps of the relative coefficient variation samples; (h) Evolution of experimental PL peak CV values; (i) J–V curves of the champion devices [45]. Copyright © 2023, John Wiley and Sons.

hidden layers and neurons is essential. By utilizing surrogate algorithms to investigate structures with up to five hidden layers, ANN-based structures facilitate precise estimation of BIPV energy outputs under realistic conditions, highlighting their potential to enhance the design and assessment of tandem PV devices. The results further indicated that regression analyses of five predictive ANN models showed a strong correlation between simulated and predicted output power, with ANN-3 exhibiting the best alignment. Furthermore, deviation analysis indicated that ANN-3 generated the most tightly clustered errors throughout both training and validation phases, substantiating its enhanced predictive accuracy relative to the other models (Fig. 3b). The results also indicated that contour plots of expected annual energy production demonstrated optimal efficiency of 4 T tandem PV cells within a bandgap range of 1.70–1.73 eV across various building orientations, necessitating various perovskite thicknesses. Their research revealed that the peak simulated power conversion performance of 31.32% was attained at a bandgap of 1.70 eV and a thickness of 780 nm under standard test conditions (Fig. 3c).

Similarly, Corcione et al. [44] designed an ML system to assess semiconductor QDs for applications in single-photon and entangled-photon quantum photonics. The emission wavelength is influenced by the size and geometry of the QDs, which regulates the quantization of its electronic phases. The random spatial and spectral variations of QDs render traditional manual selection both time-consuming and costly. They integrated conventional spectral evaluation with an autoencoding convolutional neural network to produce characteristic depictions of emission spectra. A neural network regression model utilized these characteristics to generate a suitability score and a confidence measure. The approach effectively discovered potential candidates utilizing a substantial dataset of InAs/GaAs QDs spectra, which were partially labeled by experts, while accommodating various spectral requirements and production techniques (Fig. 3d). The results further indicated that the trained autoencoder successfully reconstructed most of the test spectra, precisely identifying important peaks with minimal mistakes in the first two examples. Nonetheless, its performance deteriorated for the third spectrum owing to noise and anomalous characteristics that diverged from standard patterns. The reconstruction error was utilized as a significant feature to identify abnormalities, although the latent representations lacked definitive physical interpretability (Fig. 3e). Their work demonstrates that ML can standardize and expedite QDs evaluation, marking a significant advancement toward automated, scalable quantum photonics. Furthermore, Zhang et al. [45] designed an automated platform, SPINBOT, that incorporates ML to enhance the analysis of perovskite thin films, aiming to improve the performance of solar cells. The system uses a Bayesian optimization (BO)-based closed-loop workflow to systematically explore the intricate, high-dimensional parameter space of solution-based films. Initial studies commence with randomly selected production parameters, and each film is defined via high-throughput photoluminescence (PL) measurements. The BO algorithm evaluates these outcomes and suggests new parameter sets for future iterations, effectively directing the discovery of processing conditions. Over eight consecutive rounds, the method improved film quality, homogeneity, and reproducibility, resulting in higher PL intensity and a markedly lower coefficient of variation compared with traditional stepwise optimization techniques. The improved parameters, which include spin speed, solution quantity, dispense size, velocity, and annealing conditions, resulted in reproducible, high-quality films. Under atmospheric conditions, incorporating these films into solar cells yielded a maximum power conversion efficiency of 21.6%. Furthermore, the devices maintained 90% of their initial yield after 1100 h of continuous operation at 60–65 °C (Fig. 3f). The results further indicated that the average PL intensity initially varied but consistently increased to a peak in the final rounds, exceeding the sequential process technique. The coefficient of variation aligned closely with algorithm predictions after several iterations and continually diminished, attaining a low value of approximately 0.04, signifying enhanced uniformity and highest efficiency in the concluding phase (Fig. 3g). The results also indicated that devices constructed with the SPINBOT-optimized perovskite layer surpassed handcrafted references, attaining superior performance and enhanced photovoltaic properties. The integration of SPINBOT with BO achieved a peak efficiency of 21.6%, above that of sequential optimization. The automated method also guaranteed enhanced reproducibility and uniform performance across devices manufactured on different days (Fig. 3h, i). Their study shows that integrating robotic experimentation with advanced ML algorithms enables autonomous, high-throughput optimization of perovskite thin films, offering a scalable approach to the production of reliable, higher-performance solar cells.

3.2. Light-emitting devices

LEDs such as organic light-emitting diodes (OLEDs), QDLEDs, perovskite LEDs (PeLEDs), and laser systems play an important role in contemporary display, communication, and lighting technologies. The performance of these devices is fundamentally influenced by the properties of the emissive materials, the device design, and the production methods [46]. AI and ML offer effective methodologies for exploring this intricate parameter space. Predictive models can efficiently evaluate extensive material libraries to identify candidates exhibiting the ideal emission wavelength, quantum performance, and thermal stability [47]. Moreover, ML-based process enhancement can refine deposition parameters, layer thicknesses, and surface design, thereby reducing defects and enhancing device reproducibility. AI models facilitate the estimation of operational lifetime by analyzing degradation routes and failure modes, enabling rapid prototyping and scaling [48]. These properties collectively reduce dependence on labor-intensive experimental iterations, reduce growth phases, and expedite the conversion of innovative light-emitting materials into commercially viable devices. For example, Lin et al. [49] used ML to enhance the performance of aluminum gallium nitride (AlGaN)-based deep ultraviolet (DUV) LEDs, which often exhibit low internal quantum yields and reduced luminous output due to inherent material constraints. They used AlGaN DUV LEDs on c-plane sapphire substrates as representative devices, creating a detailed dataset encompassing both structural and electrical properties. Four ML models were trained on this dataset, with a convolutional neural network (CNN) yielding the highest accuracy, achieving an RMSE of 1.6995 W/cm^2 and a coefficient of determination (R^2) of 0.9812 for light output power density. The CNN model discovered critical features affecting device performance and demonstrated relationships between structural variables and output power that aligned with physical mechanisms and experimental findings (Fig. 4a). The results further indicated that light output power density (LOPD) attains its peak at particular levels of P1-dop, P-T, and P1—Al, with P1-dop and P1—Al having a more significant impact on LOPD than P-T. The 3D contour analysis indicated that as P1-dop increases, LOPD initially ascends due to the improved hole concentration in the p-type AlGaN layer. Nonetheless, below a specific doping threshold, an influx of impurities and defects occurs, compromising crystal integrity. These defects act as non-radiative recombination centers, reducing the efficiency of electron–hole radiative recombination and lowering light emission intensity (Fig. 4b–d). Their study demonstrates that ML can accurately predict the performance of DUV LEDs, identify essential features from complex structures, and facilitate the development of high-efficiency devices. Similarly, Choi et al. [50] designed a rule-based ML algorithm to optimize the multilayered architecture of organic LEDs to achieve precise emission colors and enhanced performance. The operation of OLEDs is significantly affected by the thicknesses and optical properties of each layer, which determine the cavity geometry and, consequently, the color and intensity of the emitted light. Conventional optimization methods are inefficient, expensive, and time-consuming due to the extensive array of potential layer combinations in multilayered systems. They developed an ML model that combines simulation analysis with two evaluation

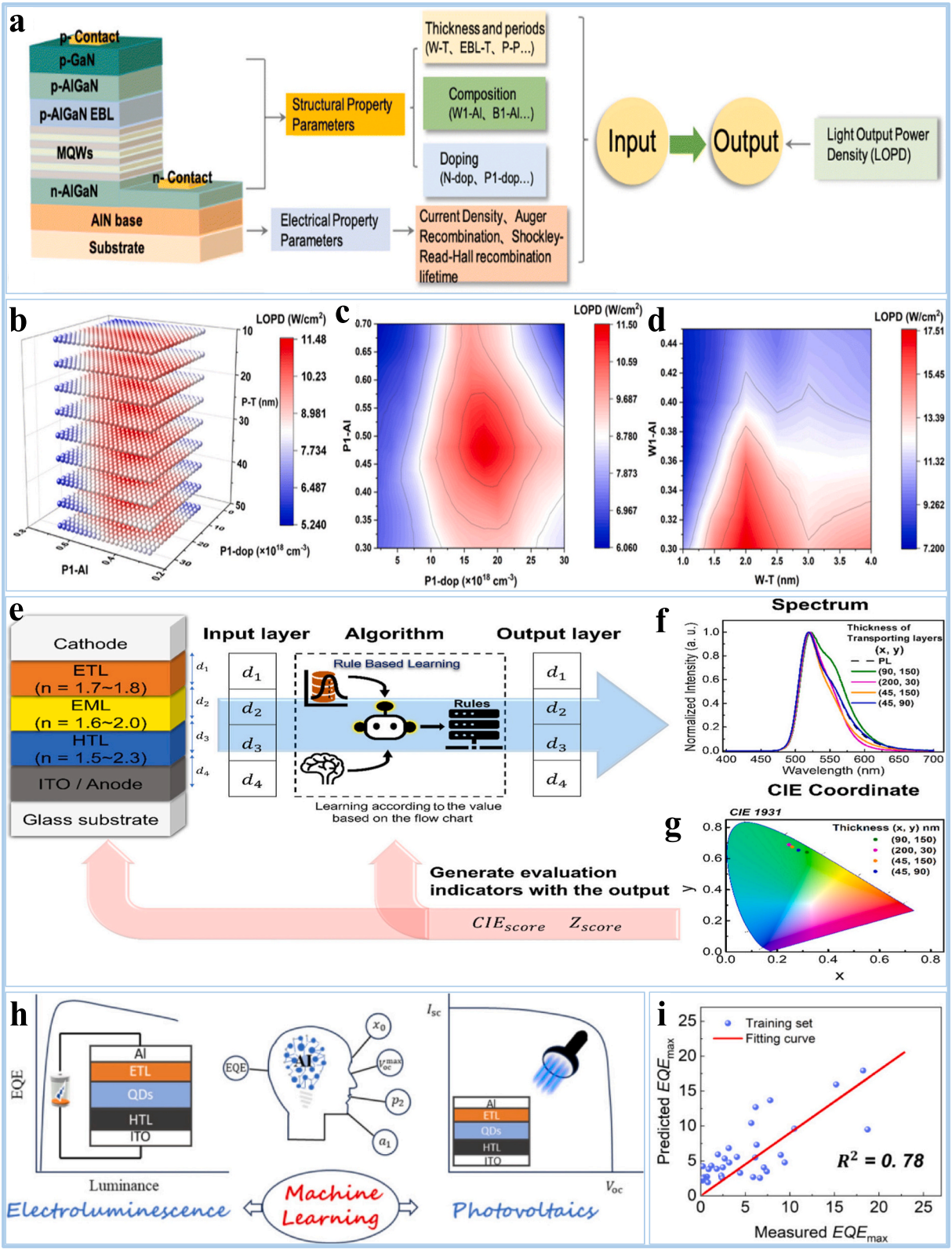


Fig. 4. (a) A preliminary input feature map: The AlGaN-based DUV LEDs' distinctive structural and electrical properties are chosen as each sample's unique properties; (b–d) Predicted LOPD with changing of different features [49]. Copyright © 2025, Royal Society of Chemistry. (e–g) An embedded block diagram demonstrates the rule-based ML process for improving the OLED design [50]. Copyright © 2024, American Chemical Society. (h) QLED analysis aided by ML; (i) Prediction results for the training and test sets, with coefficients of determination of 0.95 and 0.78, respectively [51]. Copyright © 2024, American Chemical Society.

indicators, *Z*-score and CIE-score, as dependent variables. The model systematically adjusts layer thicknesses, evaluates predicted outputs against target values, and applies established criteria to determine thickness adjustments. The process persists until the optimal device framework is achieved (Fig. 4e–g). The algorithm demonstrated high precision, achieving an error margin of less than 0.5% for red, green, and blue OLEDs. This indicates its performance in expediting OLED design, minimizing experimental workload, and delivering accurate predictions for complex multilayered optoelectronic devices. Furthermore, Yang et al. [51] utilized ML to examine the relationship between photovoltaic performance and electroluminescence in QDLEDs. They produced 123 blue and 113 green QDLEDs using various hole-transfer layers (TFB/PVK mixtures) and electron-transfer layers (ZnO: Mg with varying Mg ratios) and evaluated the devices using J–V–L measurements, photovoltaic (PV) testing, and time-resolved electroluminescence (TREL). Key metrics were gathered, including open-circuit voltage (V_{oc}) versus light intensity, short-circuit current (I_{sc}) versus light intensity, external quantum efficiency versus voltage, and TREL curves. From these, squared luminance–carrier injection rate (K^2-1) curves were calculated. Seventeen distinctive properties were derived from the observations and subsequently evaluated using decision tree and ANN models (Fig. 4h). The results further indicated that a fully connected neural network with 17 input features could precisely forecast EQE_{max} for QLEDs. Post-training, the model exhibited a robust correlation with the experimental data, with $R^2 = 0.95$ on the training set and $R^2 = 0.78$ on the test set, indicating substantial predictive accuracy and a clear relationship between the extracted features and EQEmax (Fig. 4i). Their work showed that this research deepens the physical understanding of QLEDs and offers a new approach for assessing their performance.

3.3. Photodetectors and sensors

Photodetectors and optical sensors spanning the visible, infrared (IR), and ultraviolet (UV) spectra play a vital role in imaging, optical interactions, environmental surveillance, and biomedical diagnostics. Their performance depends on intricate interactions among material properties, device formation, and environmental factors [52]. AI and ML enable systematic improvement of these devices by simulating charge transfer, photon absorption, spectral response, and noise. Algorithms based on data analysis can forecast material combinations and device geometries that enhance sensitivity, minimize response time, and broaden spectral selectivity [53]. Moreover, ML can facilitate the analysis of extensive datasets produced during device testing, revealing nuanced correlations that contribute to design enhancements and fault identification. The integration of predictive modeling with experimental feedback enhances the production of sensitive, fast, and stable photodetectors and sensors for various advanced applications [54]. Recent advancements in energy storage and conversion technologies underscore the significance of real-time characterization and structural design in enhancing device performance [55]. Specifically, in situ and operando characterization of devices based on 2D materials yields essential insights into dynamic charge transfer, interfacial behaviors, and defect evolution under operational conditions, which are equally pertinent for enhancing photodetector sensitivity, response speed, and operational stability [56]. Furthermore, novel materials investigated for advanced energy storage, including biomass-based carbon fibers and MOF-infused gel architectures, demonstrate how hierarchical porosity, adjustable surface chemistry, and improved charge-transport pathways can markedly enhance electrochemical and optoelectronic efficiency. These principles can be applied to photodetector design to improve light–matter interaction, carrier mobility, and long-term device reliability [57]. For example, Lin et al. [58] proposed an ML-assisted method to improve wavelength recognition in Cu_2O/Si self-powered photodetector arrays, facilitating advancements in image sensing technologies. A 4×4 photodetector array (PDA) was produced using a simple, economical solution-processing technique, in which p-type Cu_2O thin films were deposited on n-type Si substrates via low-power UV irradiation of Cu(II) precursor films. A UV-shielding glass plate served as a patterned mask, with unexposed areas removed by water, enabling accurate patterning without intricate lithography. The researchers employed ML algorithms to train the structure to classify and distinguish among UV, visible, and near-infrared (NIR) wavelengths based on the photocurrent responses of Cu_2O/Si heterostructures. The model correctly estimated photocurrent intensity across various wavelength ranges. This method enabled the PDA to recognize and reconstruct distinct images across different lighting conditions (Fig. 5a). The results further indicated that the Cu_2O/Si p–n junction photodetector demonstrates distinct rectifying behavior with minimal dark current. Under UV light at wavelengths below 365 nm, the photocurrent increased substantially, accompanied by a voltage change indicative of a built-in electric field, enabling self-powered functionality. The photocurrent increased with elevated UV intensity, indicating the device's heightened light sensitivity (Fig. 5b). Their findings also indicated that the band alignment of the Cu_2O/Si heterojunction facilitates broad spectral absorption from UV to NIR wavelengths and permits self-powered operation at zero bias. The large conduction-band offset promotes hole transport while impeding electron flow, thereby establishing a robust built-in potential that effectively segregates photogenerated carriers. The depth of light penetration varies with wavelength, yielding unique photocurrent responses that enable precise and reliable wavelength identification (Fig. 5c). Their research demonstrates that integrating inexpensive materials, facile production techniques, and ML-based data analysis can yield effective, multispectral, and self-powered image-sensing structures for advanced optoelectronic systems.

Similarly, Tash et al. [59] designed an ML system to predict the responsivity of photodetectors, specifically those using complex materials such as borophene. The study aimed to facilitate precise efficiency predictions before materials are prepared, given the considerable experimental challenges involved in their production. The researchers used X-ray diffraction (XRD) and Raman spectroscopy data to train ANN models, facilitating effective estimation of photodetector performance. Generative adversarial networks (GANs) were used for dataset augmentation to address data scarcity, thereby improving the model's accuracy and generalizability. Sensitivity analysis indicated that parameters such as bias voltage and spectral coefficients significantly influence device performance, consistent with experimental findings. The model forecasted the wavelength-responsivity properties of borophene-based devices on n-Si substrates, indicating peaks between 300 and 400 nm, with responsivity values spanning from 0.04 to 0.36 A/W at bias voltages of 1–5 V (Fig. 5d). This method illustrates the advantages of integrating spectroscopy data with ML methods to enhance material screening, inform experimental design, and expedite the advancement of next-generation photodetectors. Furthermore, Choi et al. [60] designed a portable capacitive photodetector that incorporates deep learning for accurate discrimination of multiple light sources, representing a significant advancement in intelligent flexible optoelectronics. The device comprises a composite structure made of silver nanowire (AgNW), zinc sulfide (ZnS)-polyurethane acrylate (PUA), and AgNW, offering mechanical flexibility and optical stability under conditions of 25% tensile strain and a bending radius of 2 mm. It demonstrates significant sensitivity at 448 and 505 nm, ensuring consistant detection performance across various deformation states and visible light conditions. The researchers utilized a one-dimensional convolutional neural network (1D-CNN) for intelligent analysis, training it on datasets of photodetector responses across different light intensities, wavelengths, and mechanical conditions. The model achieved 96.52% detection accuracy in determining light-source power levels, despite mixed signals from multiple wavelengths. This ML structure successfully extracted nonlinear trends from the photodetector's electrical response, facilitating reliable and adaptive signal interpretation (Fig. 5e). The results indicated that AgNW electrodes for stretchy electronics preserved functionality after 1000 cycles of repetitive stretching and bending.

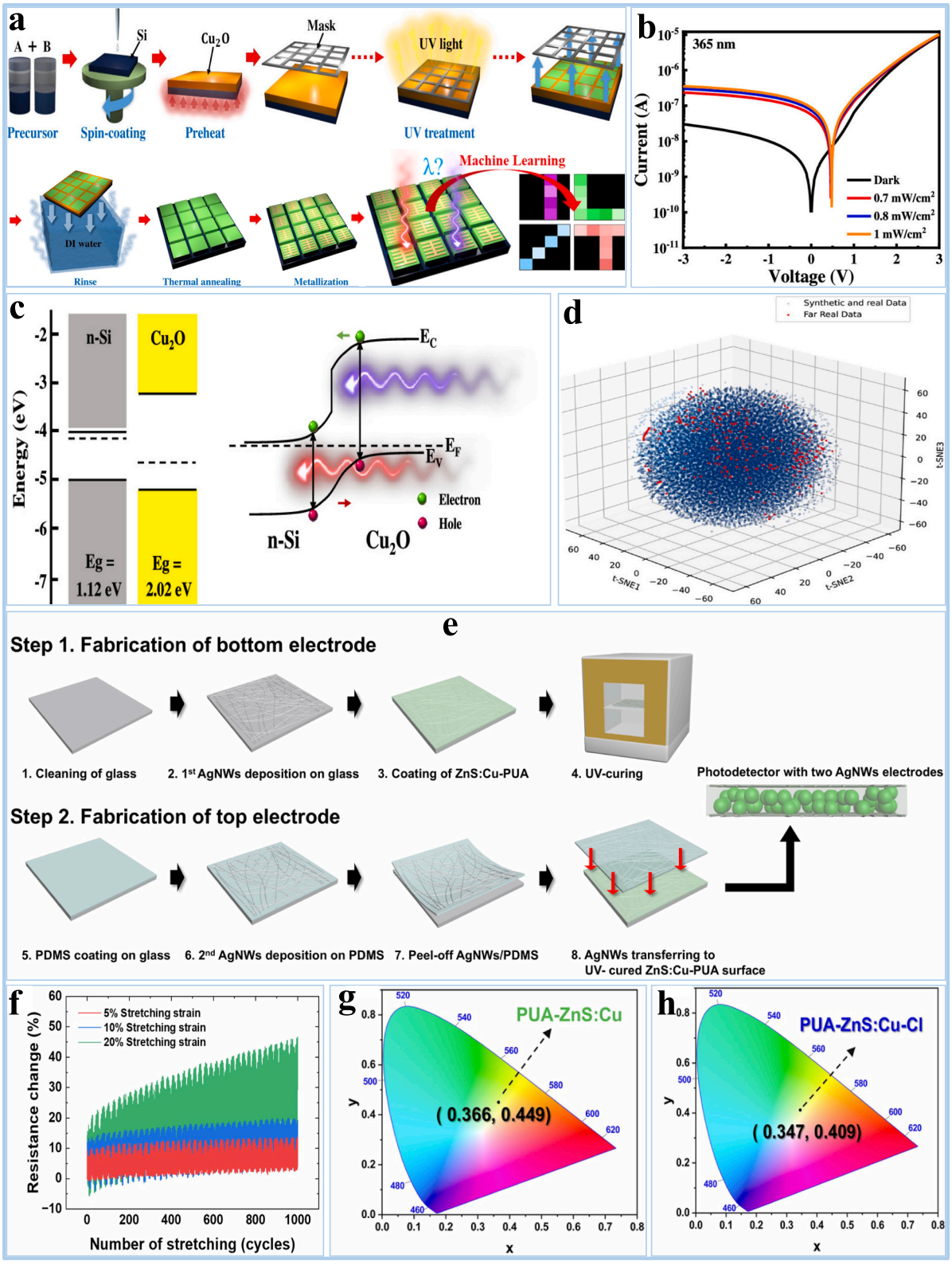


Fig. 5. (a) A schematic representation of the steps involved in creating a Cu_2O/Si PDA; (b) I − V characteristics of the representative Cu_2O/Si p − n junction photodetector; (c) Schematic diagram of the energy band alignment and corresponding band bending at the Cu_2O/Si heterojunction interface [58]. Copyright © 2025, American Chemical Society. (d) 3D visualization using an ML method that shows both generated and actual samples [59]. Copyright © 2024, John Wiley and Sons. (e) The production of a stretchy photodetector based on polymer particles; (f) Resistance variation of the top AgNWs electrode during mechanical deformation tests conducted over 1000 cycles; (g, h) Color coordinates evaluated from the measured transmission spectra, plotted on the CIE 1931 chromaticity diagram [60]. Copyright © 2025, Nature.

Resistance progressively escalated throughout the tests, and a PUA-based encapsulating layer effectively reduced electrode delamination, hence preserving device integrity (Fig. 5f). The results further indicated that the CIE 1931 color coordinates of ZnS:Cu and ZnS:Cu,Cl phosphors exhibit unique color attributes. ZnS:Cu, positioned nearer to the green spectrum, has superior performance in transmitting green light, whilst ZnS:Cu,Cl, aligned with the blue spectrum, displays heightened sensitivity to blue light. This contrast emphasizes how the specific phosphor composition affects the observed dominant wavelength and color purity, offering insight into their optical efficiency in structural color filters (Fig. 5g, h). Their study illustrates the application of ML to improve the precision and strength of optical sensing, while also laying the basis for autonomous and adaptive optoelectronic systems. AI-improved flexible photodetectors demonstrate significant potential for applications in visual light communication, smart traffic monitoring, and next-generation wearable optical sensing systems. Overall, the integration of AI-driven modeling, sophisticated characterization techniques, and information from next-generation energy materials establishes a robust foundation for the development of high-performance photodetectors and sensors, characterized by improved sensitivity, adaptability, and multifunctionality.

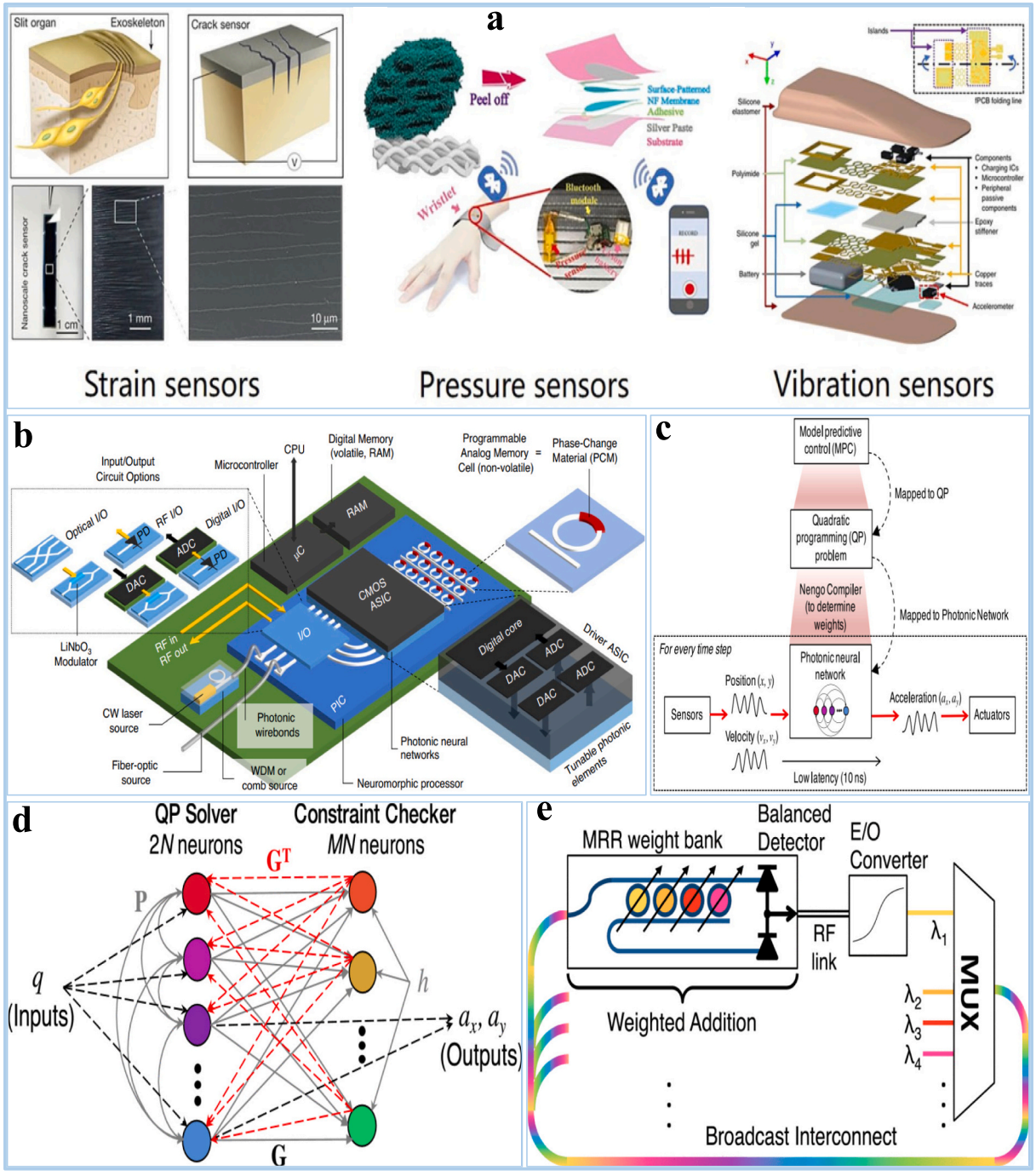


Fig. 6. (a) Typical varieties of flexible sensors [64]. Copyright © 2024, Springer. (b) A hypothetical system-in-package is illustrated, which utilizes commercially available photonic packaging technology and some emergent concepts in the field of integrated photonics [65]. Copyright © 2021, Nature. (c) A diagram showing the steps involved in putting the MPC algorithm into practice on a neuromorphic photonic processor; (d) Schematic figure of construction of a QP solver with CT-RNN; (e) Concept of an integrated broadcast-and-weight network [66]. Copyright © 2019, IEEExplore.

3.4. Next-generation optoelectronics

Emerging optoelectronic platforms, such as neuromorphic photonics, flexible electronics, and wearable devices, offer significant opportunities for developing adaptive, multifunctional devices. These technologies frequently utilize unconventional materials, hybrid structures, and intricate synthesis processes, rendering traditional design methods inadequate [61]. AI and ML facilitate the investigation of high-dimensional engineering spaces by predicting material behavior, device performance, and mechanical stability under operational conditions. In neuromorphic photonics, ML models can inform the development of photonic circuits that replicate neural computation, thereby enhancing connectivity and signal-processing efficiency [62]. In the field of flexible and wearable optoelectronics, AI helps forecast strain tolerance, energy efficiency, and environmental reliability, thereby enabling the development of devices that maintain efficiency under dynamic mechanical conditions. AI serves as a vital catalyst for advancement by minimizing experimental bottlenecks, revealing nonintuitive design solutions, and facilitating the development of next-generation optoelectronic technologies with improved functionality and versatility [63]. For example, Sun et al. [64] examined the growing significance of AI-based smart, flexible sensing devices, highlighting their essential contribution to advancing intelligent technologies. Flexible electronics are essential in dynamic contexts, including healthcare, human–computer interaction, and signal monitoring, as they facilitate accurate, adaptive, real-time data collection. The authors categorize flexible sensors into three primary types: flexible electromechanical sensors, flexible optoelectronic sensors, and flexible chemical sensors. These categories collectively establish the basis for advanced intelligent sensing devices. The integration of AI enables these devices to manage extensive and intricate datasets, thereby improving signal interpretation, predictive analysis, and adaptive responsiveness. The integration of flexible sensing and AI facilitates the development of more intelligent, autonomous, and contextually aware wearable technologies (Fig. 6a). Flexible electromechanical sensors are essential for transforming mechanical stimuli, such as pressure, strain, vibration, and shear stress, into electrical signals. Composed of materials including metal nanoparticles, metal oxides, carbon nanomaterials, liquid metals, conductive polymers, and transition metal dichalcogenides, these structures can bend and conform to intricate surfaces. These properties render them suitable for applications in wearable devices and soft robotics, where flexibility and sensitivity are critical. High-sensitivity strain sensors exhibit gauge factors (GFs) exceeding 5000, a lower detection limit (strain $<1\%$), and fast response times, enabling the collection of subtle physiological signals, such as pulse, heartbeat, and throat vibrations, for applications in speech recognition and pronunciation calibration. Sensors that exhibit larger strain ranges are advantageous for motion tracking, as they can detect movements including finger, wrist, or knee bending. This capability facilitates applications such as gesture translation, Braille reading, and assistive control devices. The integration of AI algorithms with these sensors enables the intelligent processing and interpretation of complex mechanical signal patterns, thereby improving accuracy, adaptability, and self-calibration. Similarly, Shastri et al. [65] provide a thorough study of the emerging field of photonic computing and neuromorphic systems, emphasizing their capacity to revolutionize AI and ML applications. The increase in optoelectronic components in photonic integration devices has enabled the development of photonic integrated circuits (PICs) capable of executing ultrafast ANN computations. These devices leverage the high-speed properties of light to analyze data significantly faster than traditional electronic hardware, while ensuring energy reliability. The authors highlight that an algorithm executed on photonic hardware can meet the growing computational requirements of AI across various fields, including medical diagnostics, telecommunications, scientific computing, and real-time data analytics. The study examines the concurrent advancement of neuromorphic electronics, aiming to replicate the architecture and functionality of biological neural networks to improve AI performance (Fig. 6b). Neuromorphic electronic devices encounter considerable limitations, especially regarding processor latency; however, neuromorphic photonics presents an intriguing complementary alternative. Photonic neuromorphic devices operating at sub-nanosecond speeds significantly reduce latency and maintain parallel computation, thereby facilitating real-time and large-scale AI processing. Furthermore, Lima et al. [66] present a detailed tutorial on neuromorphic photonic devices and their prospective applications in ML and AI. Neuromorphic photonics leverages the intrinsic benefits of light-based computing, including ultrafast signal propagation, parallelism, and reduced energy dissipation, to achieve efficiency that surpasses that of traditional digital electronics. These devices are capable of performing intricate computations for ML tasks, such as optimization, control, and deep learning inference, achieving significant enhancements in speed and energy efficiency. They outline device examples and the physical principles necessary for the practical design of neuromorphic photonic hardware, including integrated photonic circuits, optical neurons, and synaptic weight modulation. Simulating and implementing such devices enables AI algorithms to operate with sub-nanosecond latencies, facilitating fast learning and inference. This capability is especially beneficial for real-time applications in autonomous networks, telecommunications, scientific computing, and data-intensive analytics (Fig. 6c). They further revealed that the nonlinear programming challenge in model predictive control was executed utilizing a 24-neuron network proficient at managing a three-step prediction horizon. The network was segmented into two factions: one expressing control variables and the other imposing system limits. Utilizing fixed and variable weights and biases associated with system matrices and constraints, the network dynamically imposed boundary conditions, enabling the control neurons to converge on the optimal solution (Fig. 6d). The results also indicated that neuromorphic photonics amalgamates optical and electrical processing to attain high throughput, scalability, and reconfigurability via an O/E/O system. This method involves multiplexing and weighting optical signals, converting them into electronic photocurrent, and subsequently using the resulting photocurrent to drive optical outputs. This notion led to the design of the broadcast-and-weight architecture, which facilitates efficient signal processing through components such as microrings (Fig. 6e). Their work showed that integrating neuroscience-inspired structures with photonic hardware establishes a novel paradigm for high-speed, energy-efficient AI computation, effectively connecting theoretical ML structures with practical hardware implementation. In addition, a comparative analysis across optoelectronic devices reveals that photovoltaic studies primarily focus on efficiency and stability prediction using structured datasets, while LED research emphasizes spectral tuning and emission control using deep learning models (Table 1). In contrast, photodetectors rely heavily on signal-processing-driven ML approaches, where real-time classification and noise reduction are important. This cross-device comparison highlights that algorithm selection is strongly dependent on data type, with structured material descriptors dominating photovoltaics, and time-series or spectral data being more relevant for photodetectors and LEDs.

4. ML and AI in energy storage devices

The rapid shift to renewable energy sources requires high-performance, reliable, and cost-effective energy storage devices. Batteries and supercapacitors are essential components in managing energy supply and demand, facilitating electric mobility and enhancing the stability of renewable energy grids [67]. The design and improvement of storage materials pose complexities arising from complex relationships among structure, chemistry, electrochemical activity, and degradation processes [68]. ML and AI have become significant tools for advancing innovation in this domain. These methods facilitate the estimation of material properties, the identification of promising electrode and electrolyte candidates, and the enhancement of device building blocks by

Table 1
Cross-comparison of ML approaches in optoelectronic devices.

Materials	Device type	ML/AI algorithm	Input features	Target metrics	Key performance	Key insight	Ref.
Halide perovskites	Photovoltaic	RF, ANN	Composition, bandgap	PCE, stability	>90% accuracy	Rapid screening	[28]
Organic semiconductors	Photovoltaic	GB	Molecular descriptors	PCE, mobility	Improved selection	Structure-property link	[46]
Quantum dots	LED	NN	Size, ligands	Emission wavelength	Precise tuning	Color control	[49]
Perovskite NCs	LED	DL	Spectral data	Luminescence	High reliability	Defect insights	[50]
Cu_2O/Si	Photodetector	Supervised ML	Photocurrent	Wavelength	Accurate detection	Multi-spectral	[58]
Borophene	Photodetector	ANN, GAN	XRD, Raman	Responsivity	0.04–0.36 A/W	Data augmentation	[59]
AgNW/ZnS	Photodetector	CNN	Electrical signals	Accuracy	96.52%	Robust sensing	[60]

extracting trends from extensive experimental and computational datasets [69]. In addition to materials discovery, AI and ML techniques have demonstrated their utility in modeling charge–discharge behavior, predicting capacity fade, and enhancing safety and performance by leveraging data-driven insights [70]. Across these studies, datasets ranged from several hundred to over 74,000 entries, depending on the material type and property. Validation was performed using independent test sets, k-fold cross-validation, or transfer learning, depending on the study. Baseline comparisons included conventional regression models, graph neural networks (GNNs), or physics-informed models, providing clear reference points for reported metrics such as R^2, RMSE, and percentage improvements. These details ensure that performance metrics are interpretable, reproducible, and grounded in rigorous evaluation practices. This section specifies the increasing significance of ML and AI in the development of energy storage devices. It encompasses applications across various types of batteries, including lithium-ion, sodium-ion, solid-state, and multivalent systems, as well as supercapacitors and hybrid devices. The text emphasizes the importance of data-driven strategies in material exploration and predictive modeling techniques that are transforming the design and development of next-generation energy storage technologies.

4.1. Batteries

Rechargeable batteries are a fundamental component of contemporary energy storage solutions, powering a wide range of applications, including portable electronics, electric vehicles, and grid systems [71]. Lithium-ion batteries currently dominate the market; however, issues related to resource availability, safety, and cost have prompted exploration into alternative technologies, including sodium-ion, solid-state, and multivalent devices [72–74]. Next-generation batteries offer potential benefits in energy density, stability, and sustainability; however, their development and optimization pose challenges due to intricate electrochemical and interfacial phenomena [75]. ML and AI are used to enhance electrode and electrolyte development, improve production parameters, and forecast performance metrics such as voltage, capacity, and cycling stability. ML and AI facilitate the accelerated, more precise development of high-performance battery chemistries by analyzing large experimental and computational datasets [76]. For example, Meng et al. [77] performed an extensive investigation into the development of cathode materials for sodium-ion batteries utilizing AI. They introduced a novel graph deep learning algorithm referred to as the multivalent metal-ion battery voltage graph neural network (MBVGNN). Standard deep learning algorithms used in battery studies primarily rely on fundamental or topological data, often overlooking the geometrical arrangement and global structural details necessary for accurate voltage prediction. MBVGNN addresses this limitation by integrating the missing properties, which enables it to capture the intrinsic physical and chemical interactions that govern electrochemical processes more effectively. The model achieved $R^2 = 0.969$ for formation energy prediction and showed a 43.98% enhancement compared to GATGNN and a 47.06% increase relative to TL-CGCNN on the sodium-ion battery dataset. The voltage prediction precision for multivalent metal-ion structures, specifically Ca, Zn, Al, and Mg, has been improved, showing enhancements of 15.50%, 28.09%, 44.74%, and 18%, respectively. Additionally, MBVGNN demonstrated an effective prediction of the formation energy of cathode materials, achieving an R^2 value of 0.969, which validates its reliability in evaluating thermodynamic stability (Fig. 7a). The authors further conducted DFT calculations on 222 nickel-based sodium-ion cathode materials to verify the model, with an emphasis on high-nickel ternary structures. The strong correlation observed between MBVGNN predictions and DFT results validates the model's reliability and practical applicability. The study conducted large-scale screening, identifying 194 high-energy-density sodium-ion cathode candidates. This outcome underscores the method's efficiency in identifying fast materials. Furthermore, MBVGNN demonstrated the ability to predict the average voltage of fluorine-substituted layered oxide cathodes, a category of materials with favorable energy storage properties. Based on the predictive accuracy achieved, the researchers developed a comprehensive dataset comprising 74,553 high-entropy cathode materials, including layered oxides and a range of polyanionic structures. Based on the data, knowledge-guided insights were derived regarding 16 key material classes, prioritized elemental combinations, and over 1.3 million potential compositional variations pertinent to experimental synthesis (Fig. 7b). Their results showed that parallel set graphs were used to visualize the data distribution of high-entropy datasets in relation to the target correlation structure, highlighting trends that support the design of multi-doped high-entropy materials with enhanced redox potential (Fig. 7c). Their study demonstrates that AI-driven, graph-based deep learning is an effective method for enhancing the discovery and development of cathode materials with elevated voltage and high energy density. This structure offers a systematic approach to inform future multi-doping methods, facilitating the integration of computational predictions and experimental validation in advancing next-generation sodium-ion batteries.

Similarly, Carvalho et al. [78] combined AI with quantum mechanical simulations to screen a molecular library of 74,553 organic molecules, predicting energy densities and voltages for lithium-ion cathodes. The system addresses the difficulties of energy density, rate efficiency, and cycling durability that currently hinder the adoption of organic electrode materials (OEMs). Their methodology combines AI with quantum-mechanical simulation to facilitate systematic, high-throughput screening of extensive molecular libraries, thereby expediting the rational development of high-energy, sustainable cathodes. This structure incorporates the simplified molecular-input line-entry system (SMILES) as a text-based molecular fingerprint. Processing is conducted using a hybrid neural network architecture that integrates recurrent neural networks (RNNs) with fully connected neural networks (FCNNs). The SMILES strings undergo tokenization into smaller fragments, facilitating the formation of a unique molecular vocabulary. These fragments then transform into index-based visualizations, which are subsequently converted into embedding vectors. The embeddings enable the network to acquire the chemical significance of atoms, bonds, and molecular substructures, thereby effectively collecting the structure–property interactions pertinent to cathode efficiency. This approach diverges from earlier techniques that used SMILES for molecular generation or topological analysis, focusing instead on direct property prediction based on molecular arrangement (Fig. 7d). The researchers identified 459 new OEM candidates with potential energy densities greater than 1000 Wh kg^{-1} using this hybrid AI-quantum

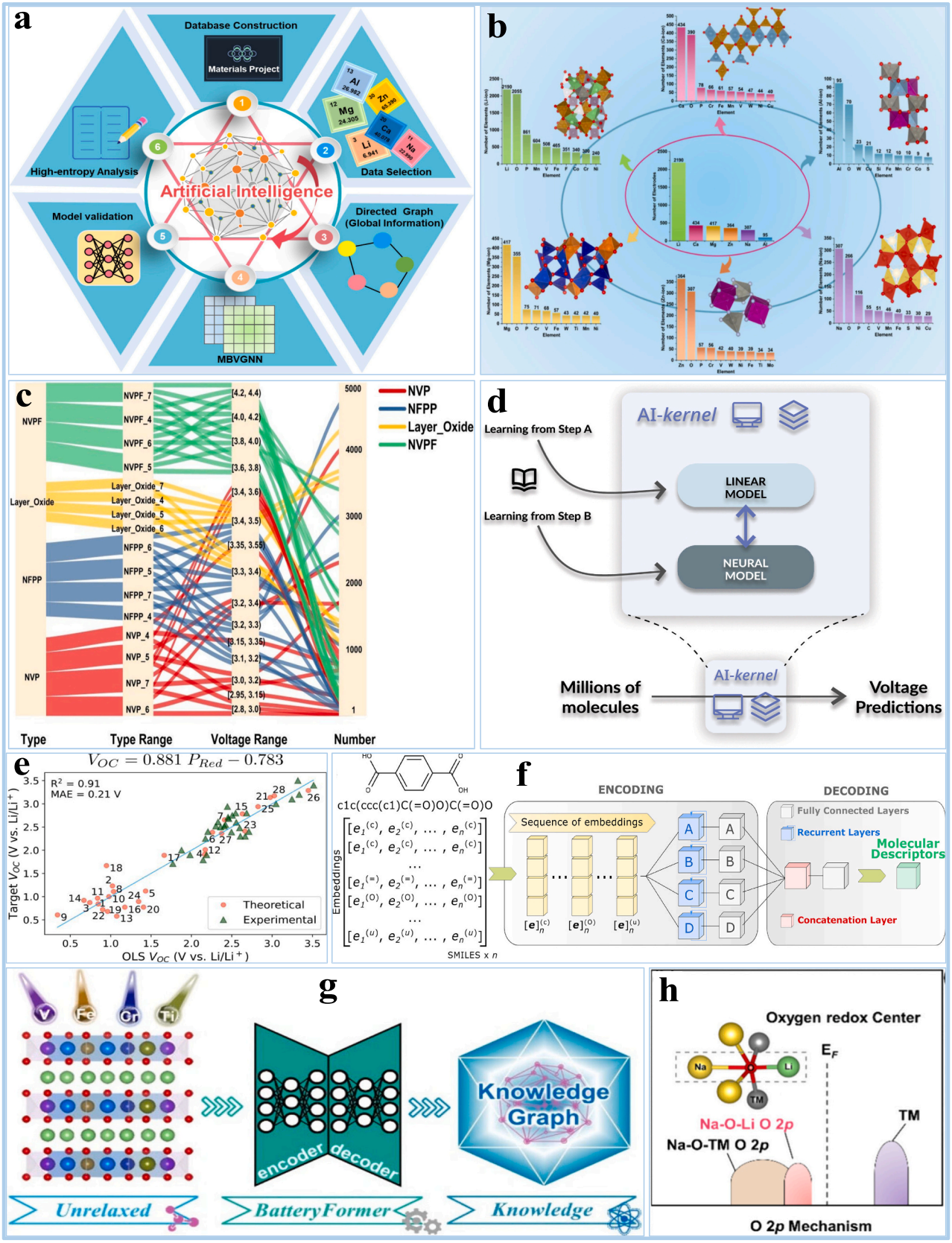


Fig. 7. (a) Graphical representation of AI-driven cathode material synthesis for sodium-ion batteries; (b) Distribution of the numbers of battery materials collected from the material project database; (c) Parallel set graph of four kinds of high entropy cathode materials [77]. Copyright © 2024, Elsevier. (d) An illustration of the AI kernel's working concept; (e) The OLS model connecting the reduction potential molecular descriptor and the open-circuit voltage; (f) Neural network schematic showing SMILES converted into embedding vectors as input [78]. Copyright © 2022, Elsevier. (g) Graphical illustration of a universal ML structure that is driven by AI for the development of ion battery cathode materials; (h) Illustration of the oxygen redox center mechanism [79]. Copyright © 2025, American Chemical Society.

approach. The model identified significant molecular properties, such as a donor–acceptor-like impact, which enhances electrode voltages and informs future molecular development strategies. Their findings indicated that the regression model demonstrated robust consistency between predicted and actual voltages, especially for experimental data. The neural network encoded molecular structures from SMILES using embeddings and RNN layers, then decoded structure–property connections through fully connected layers, thereby demonstrating reliable performance in predicting reduction potentials (Fig. 7e). Their result also indicated that the trained AI structures facilitated ultra-rapid high-throughput screening of 20 million compounds from the GDB17 dataset, predicting lithiation voltages in less than 40 min on a personal computer. The use of voltage and capacity filters yielded a limited selection of potential candidates, comprising 1001 cathodes and a more extensive array of anodes (Fig. 7f). Their study also evaluated various molecular representations, including the Coulomb matrix (CM) and the many-body tensor representation (MBTR), within multiple deep learning systems. This evaluation highlighted the successful application of text-based molecular encoding in predictive modeling. Their work demonstrates the integration of AI, natural language processing-based molecular encoding, and quantum simulations to enhance the discovery and enhancement of high-performance, renewable organic cathode substrates. It offers a structured approach for advancing the next generation of environmentally friendly lithium-ion batteries. Furthermore, Meng et al. [79] developed Battery-Former, a comprehensive ML system designed to enhance the discovery and development of ion battery cathode materials. Conventional graph neural networks used for predicting crystal properties generally require accurate atomic positions and types, thereby limiting their applicability to new or theoretical materials. Battery-Former addresses this limitation by using average interatomic radii as edge embeddings rather than precise bond lengths. This approach facilitates fast, high-throughput screening that relies solely on material composition and structural design. This method is especially effective for investigating novel chemical environments and developing advanced battery materials. Battery-Former further exhibits strong predictive capabilities across various cathode chemistries. The model provides precise predictions of elevated redox potentials for layered oxides, fluorophosphate salts, vanadium fluorophosphate salts, and ferric pyrophosphate salts. Additionally, it accurately forecasts the small redox potential of Na_6CoS_4 at 1.56 V. The model not only provides numerical predictions but also identifies important local structural motifs, including the linear $Na - O - Li$ structure found in layered transition metallic oxides, which play an important role in improving redox functionality. The capacity to generalize across various lithium-ion battery cathode materials highlights its adaptability and dependability (Fig. 7g). The results further showed that an investigation of the premier high-voltage high-entropy structures demonstrated a significant correlation between elemental frequency and redox potential, with lithium being the most prevalent, followed by calcium. Elements with greater electron-donating capacity were more abundant, thereby improving redox efficiency. The results also illustrated the model's capacity to capture local structural properties, enhancing interpretability and correlating effectively with experimental trends (Fig. 7h). This approach effectively connects computational estimations with experimental validation, thereby facilitating advancements in next-generation high-energy-density batteries.

4.2. Supercapacitors and hybrid devices

Supercapacitors serve as an intermediary between traditional capacitors and batteries, providing fast charging and discharging, extended cycle life, and high power density. Nonetheless, the comparatively low energy density remains a limitation [80]. Hybrid energy storage devices that integrate battery-like faradaic reactions with capacitor-like charge storage are emerging as a viable choice [81,82]. The development of these devices relies on the optimization of electrode materials, electrolyte composition, and interfacial dynamics, all of which encompass multidimensional variables [83]. ML and AI offer robust methodologies for analyzing these factors, predicting electrochemical conduct, and directing the production of advanced nanostructured materials. Recent studies demonstrate the capacity of data-driven models to increase capacitance, enhance ion transport, and improve the overall energy–power balance of supercapacitors and hybrid devices [84]. For example, Park et al. [85] conducted an in-depth investigation into the performance forecasting of hybrid energy harvesting devices (EHDs) that combine photovoltaic cells (PVCs) with thermoelectric generators (TEGs), using ML algorithms to evaluate and enhance device efficiency. They trained 8 ML models on experimental data from 5 hybrid EHDs and used 11-fold cross-validation. ANN models achieved $R^2 = 0.944–0.962$ for the test set, outperforming other models (Fig. 8a). The authors investigated data-driven modeling to establish correlations between material properties, design variables, and output functionality. Eight distinct ML models were trained and assessed utilizing experimental data from five EHDs arrangements, each characterized by a unique interface material between the PVC and TEG components. To achieve strong predictive performance and reduce overfitting, the dataset was split into 11 folds using 11-fold cross-validation. In each fold, 10 subsets were used for training, and 1 for testing, with this process repeated 11 times to ensure each subset served as a test set exactly once. Model evaluation metrics included the coefficient of determination (R^2), RMSE, and mean absolute error (MAE), providing a comprehensive assessment of predictive accuracy. Higher R^2 values and lower RMSE and MAE values indicate a more efficient model. The findings indicated that the ANN consistently outperformed all other models, achieving R^2 values of 0.962 on the training set and 0.944 on the test set. The RMSE values for all three output variables (T_1, T_2, and V_S) were below 3.0, whereas other models demonstrated higher RMSE for at least one output, suggesting lower predictive precision (Fig. 8b). The negligible efficiency disparity between the training and test sets indicates the lack of overfitting, underscoring the ANN's capacity for efficient generalization across various EHDs arrangements. The ANN structure included two hidden layers utilizing ReLU activation functions, processing input variables via weighted sums to produce predictions for the output variables. This structure enabled the system to identify intricate, nonlinear correlations between surface material properties and device performance. The authors showed that an EHD with a carbon-paste interface achieved 2.6% higher output power at 1000 W/m^2 irradiance than a standalone PVC, highlighting the practical advantages of ML in enhancing integrated energy systems. Their study demonstrates the successful use of ANN-based ML to predict and improve the efficiency of EHDs (Fig. 8c–e). This method effectively correlates input variables with output behavior, serving as a valuable resource for material selection, interface development, and device design, thereby expediting the advancement of high-performance, multifunctional energy systems. Similarly, Mursal et al. [86] investigated the development and enhancement of MnO_2-based supercapacitors (SCs) using ML, focusing on the limitations of conventional experimental approaches. MnO_2 is recognized as a potential electrode component for supercapacitors, attributed to its outstanding theoretical capacitance, availability, and cost-effectiveness. Enhancing production, synthesis, and electrochemical testing conditions to achieve high performance is time-intensive and resource-demanding, often restricting systematic investigation of essential variables such as structure, crystal phase, and electrolyte relationships. To address these challenges, the authors assembled a detailed dataset of around 5000 chemical entries, including synthesis settings, electrode production parameters, and electrochemical efficiency metrics. The researchers utilized classification and regression tree (CART) evaluation to derive interpretable selection rules, facilitating the determination of the key features influencing specific capacitance, cyclic stability, and capacitance retention. Feature importance evaluation facilitated the prioritization of essential factors, and forecasting models were constructed employing

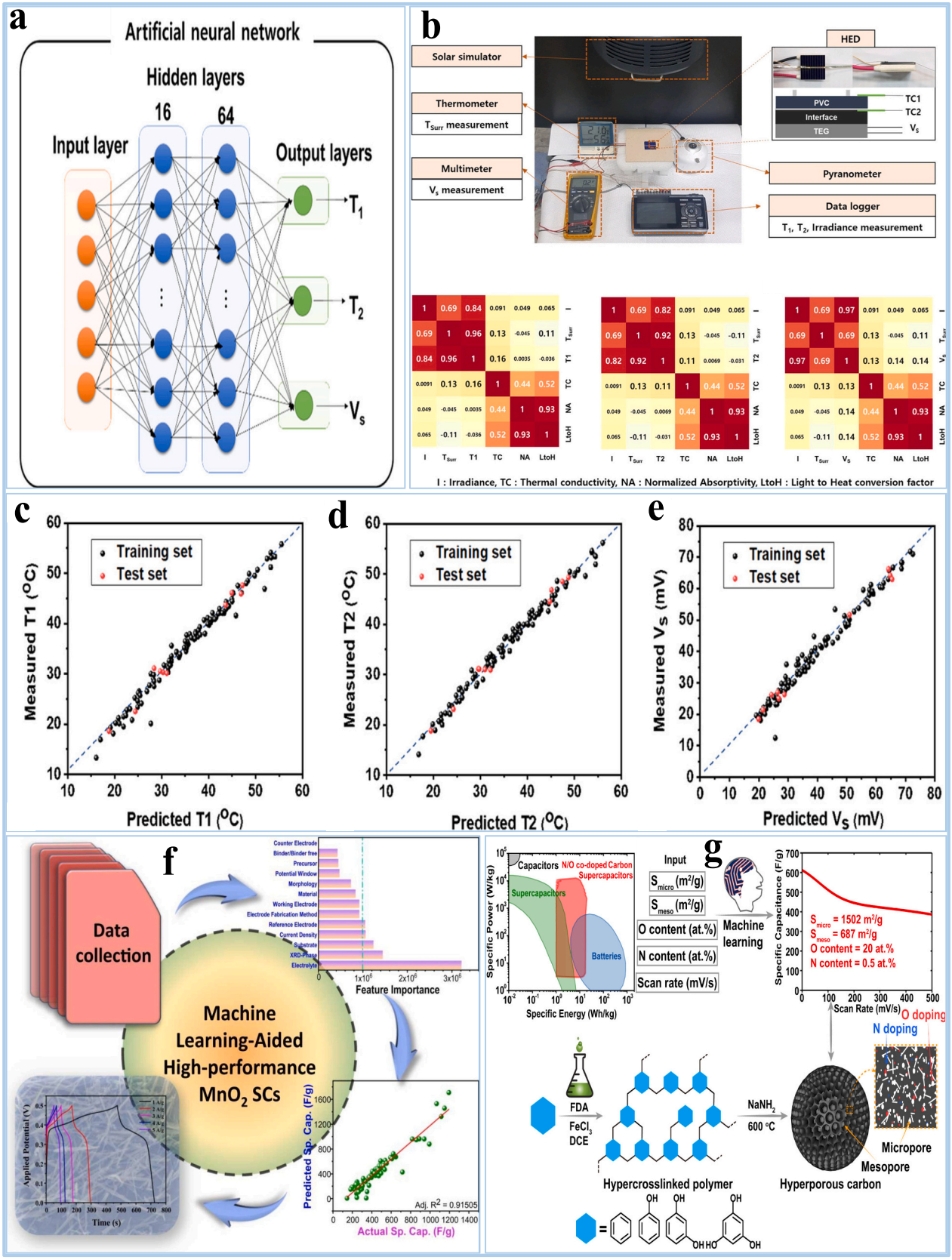


Fig. 8. (a) A scheme of the ANN, including parameters and nodes; (b) Photograph of our experimental setup and the correlation matrices of T_1, T_2, and V_S; (c–e) Their corresponding linear correlation between the true and predicted results [85]. Copyright © 2022, American Chemical Society. (f) Schematic representation of an ML-based method for MnO_2 SC prediction and optimization [86]. Copyright © 2025, Elsevier. (g) Synthesis of hyperporous carbons for supercapacitors using ML [87]. Copyright © 2023, Nature.

various ML algorithms to establish correlations between input variables and supply chain performance. The random forest algorithm demonstrated the highest predictive precision among the models, successfully capturing nonlinear relationships between material and computation variables and efficiency outcomes. The experimental validation of ML insights was achieved by producing MnO_2 electrodes under the CART-optimized conditions. The supercapacitors exhibited notable functionality, attaining a specific capacitance of 498 F/g, a coulombic yield of 95.52%, and remarkable cyclic stability with 84.12% capacitance retention after 10,000 cycles. The results validate the predictive capabilities of the ML-driven method and underscore its potential to enhance experimental development efficiency (Fig. 8f). Their study demonstrates the performance of data-driven approaches in enhancing the discovery and improvement of high-performance batteries. Their work also integrates large datasets with interpretable ML models to establish a structure for systematically discovering optimal material formulations, processing conditions, and testing parameters. This approach facilitates the rational development of next-generation MnO_2-derived supercapacitors, enhancing their performance and longevity. Furthermore, Wang et al. [87] examined the ML-assisted development of highly porous, oxygen-enriched carbon materials for aqueous supercapacitors, highlighting the constraints of conventional experimental methods, which are often time-consuming and resource-intensive. Porous carbons serve as effective supercapacitor electrodes owing to their outstanding electrical properties, long-term cycling stability, and broad operating temperature range. However, optimizing their physicochemical and electrochemical properties requires a systematic investigation of the pore structure, surface chemistry, and doping levels. The authors further employed ML to analyze literature data and identify essential features for the development of high-performance carbon electrodes, thereby expediting the process. Utilizing these insights, an activation approach was formulated using sodium amide and cross-linked polymer precursors, yielding highly porous carbons with specific surface areas exceeding 4000 m^2/g. By adjusting pore size and oxygen content, the electrodes, with a mass loading of 0.7 mg/cm^2, exhibited a specific capacitance of 610 F/g in 1 M H_2SO_4, which closely aligns with ML predictions (Fig. 8g). Complementary investigations into charge storage processes and electrolyte transport, using step-potential electrochemical spectroscopy and quasielastic neutron scattering, further validated the impact of structural properties on performance. They further utilized an ANN to forecast the electrochemical activity of N/O co-doped activated carbon electrodes. The ANN was trained on 288 data points encompassing micropore and mesopore surface areas, nitrogen and oxygen doping amounts, and cyclic voltammetry scan rates, while the electrolyte type (6 M KOH or 1 M H_2SO_4) was treated as a categorical variable. The model, employing a single hidden layer of 7 neurons with hyperbolic tangent sigmoid activation and Bayesian regularization, demonstrated strong performance, yielding RMSE values of 25.0, 34.5, and 38.5 on the training, validation, and test datasets, respectively. The ANN studies further indicated that specific capacitance improves with oxygen levels, achieving maximum predicted efficiency at micropore and mesopore surface areas of 1502 and 687 m^2/g, respectively, with 0.5 at.% nitrogen doping and 20 at.% oxygen doping. The model indicated that excess oxygen doping in 1 M H_2SO_4 enhances electronic conductivity and electrode wetting, thereby improving capacitance. Their studies collectively demonstrate that integrating ML, ANN-based forecasting, and targeted experimental design establishes a quantitative structure to enhance porous carbon electrodes, facilitating the discovery of high-performance N/O-codoped materials for next-generation supercapacitors.

4.3. Data-driven electrode & electrolyte discovery

The properties of the electrode and electrolyte materials utilized predominantly influence the operational features of energy storage devices. Conventional discovery techniques rely on lengthy experimentation; however, contemporary data-driven methodologies enable rapid screening and systematic design [88]. ML and AI tools analyze extensive materials databases and simulation results to forecast properties, including ionic conductivity, electrochemical stability, and redox potential [89]. The insights enable researchers to pinpoint promising material candidates before synthesis, significantly reducing development cycles. The integration of experimental data with high-throughput calculation and ML has facilitated the discovery of novel electrodes and electrolytes specifically designed for various storage technologies [90]. For example, Nair et al. [91] emphasized the growing significance of AI and ML in the development of next-generation battery electrolytes. They screened >40,000 electrolyte molecules, validated predictions with cross-validation, and benchmarked results against conventional regression approaches (Fig. 9a). Electrolytes play a vital role in battery safety, electrochemical performance, and operational longevity; however, traditional trial-and-error methods for their production tend to be time-consuming, resource-intensive, and inefficient. AI and ML offer data-driven methodologies that enhance screening, prediction, and optimization of electrolyte materials, facilitating a more systematic and focused investigation than traditional approaches. Their study utilized both supervised and unsupervised ML methods. Supervised learning used labeled data for regression and classification tasks with models including linear regression, support vector machines, decision trees, and random forests. Unsupervised learning was applied to unlabeled datasets for tasks such as clustering and dimensionality reduction, using approaches including k-means clustering, hierarchical clustering, principal component analysis (PCA), and Gaussian mixture models. The performance and generalization of these models depended significantly on the quantity and quality of training data, obtained from experimental measurements and computational simulations. Publicly accessible repositories such as the Materials Project, Organic Materials Database, and Inorganic Crystal Structure Database served as a substantial basis for model training, verified by their research. They further employed ML models to analyze essential electrolyte parameters, including chemical composition, solvent selection, and salt concentration, revealing correlations and trends that are challenging to discern experimentally. Initial research focused on predicting essential electrolyte properties, while later investigations expanded to the design of electrolytes with customized properties tailored to specific battery chemistries. Generative models were used to identify new electrolyte candidates with enhanced ionic conductivity, electrochemical stability, and electrode compatibility. Their study illustrates that AI and ML can serve as transformative tools to enhance the rational design of safe, effective, and green next-generation battery electrolytes, thereby facilitating faster, more systematic discovery of high-performance energy storage materials. Similarly, Alzaabi et al. [92] designed an AI-driven structure to expedite the development of sodium-ion battery (SIB) electrode materials, recognized as a viable alternative to lithium-ion batteries owing to the abundance, cost-effectiveness, and safety benefits of sodium. The development of outstanding SIB electrodes poses challenges due to complex interactions between compositional and structural features that influence key properties, including specific capacity, average voltage, and volumetric capacity. Their research involved training four ML algorithms: decision tree, random forest, support vector machine (SVM), and DNN on a dataset enriched with features obtained from high-throughput computational databases. The DNN model demonstrated the greatest predictive accuracy, achieving R^2 values of up to 0.97 and mean absolute errors of less than 0.11 for the target characteristics. To facilitate material selection, DNN predictions were combined with the Non-dominated Sorting Genetic Algorithm II (NSGA-II) to identify Pareto-optimal electrode materials that optimize specific capacity while minimizing volume change. The chosen candidates exhibited balanced electrochemical performance, underscoring their suitability for practical SIB applications. This method further highlights improvements in battery efficiency for enhanced energy storage solutions. The results showed that by tailoring capacity and

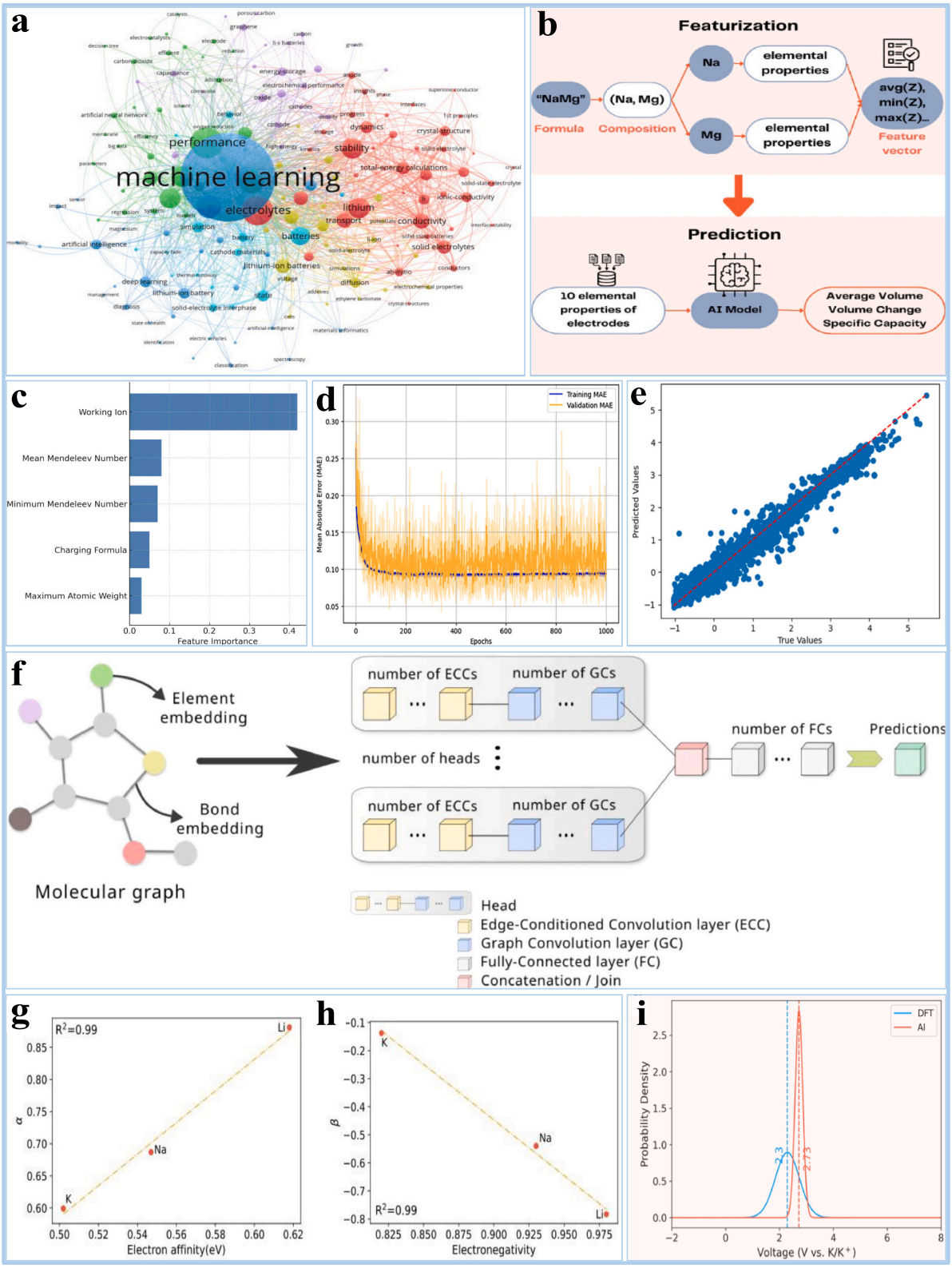


Fig. 9. (a) A schematic illustrating the multifaceted application of ML in the production of battery electrolytes through the use of a keyword co-occurrence algorithm [91]. Copyright © 2025, AIP Publishing. (b) A graphical representation of the process of advancing the synthesis of sodium-ion electrode materials through AI-driven optimization and predictive modeling; (c) Decision tree feature importance for voltage prediction; (d) DNN learning curves showing training and validation errors; (e) Scatter plots comparing DNN predicted and actual values [92]. Copyright © 2025, Elsevier. (f) Schematics depicting the entire RSNM; (g, h) Linear model performance for Na and K batteries with parameter correlations; (i) PDF comparison of AI and DFT results for reduction potentials and open-circuit voltages [93]. Copyright © 2023, Elsevier.

volumetric growth, batteries can be engineered for various applications, including electric vehicles, wearable electronics, and sustainable energy storage devices. The NSGA-II-based multi-objective optimization establishes a search space using scaled battery feature data and employs real random sampling, simulated binary crossover, polynomial mutation, and energy-based reference directions to effectively investigate trade-offs among performance metrics. Their case study further examines the utilization of grid energy storage systems (GESS) within the proposed structure. The growing integration of renewable energy necessitates reliable, flexible, and efficient storage solutions for GESS. The optimized results revealed four potential solutions, each illustrating unique trade-offs between specific capacity and volumetric growth, with increased tolerances limited to 30% and a focus on higher capacities for improved productivity. Mapping these trade-offs facilitates informed material choices and design, thereby substantially minimizing the dependence on experimental trial-and-error approaches (Fig. 9b). The results further showed that feature importance analysis of the decision tree identified the working ion as the primary factor governing voltage prediction, followed by Mendeleev number descriptors, charging formula, and maximum atomic weight. These chemically meaningful features enabled the model to distinguish materials while maintaining both interpretability and predictive accuracy systematically (Fig. 9c). The results also showed that the DNN model achieved the highest predictive accuracy for specific capacity, outperforming random forest, SVM, and decision tree models. While the learning curve indicated strong initial learning, later divergence between training and validation errors suggested overfitting, which was mitigated using dropout and L2 regularization (Fig. 9d). The results further showed that the DNN model maintained strong predictive performance, with low error and high accuracy. The close alignment between predicted and actual values confirmed its reliability for specific capacity prediction (Fig. 9e). Their study shows that deep learning and multi-objective evaluation can accelerate the identification of next-generation sodium-ion electrode materials, leading to high-performance, cost-effective, and application-specific energy storage solutions. Furthermore, Carvalho et al. [93] developed an evolutionary AI-driven structure to expedite the identification of redox-stable organic electrode materials for Li-, Na-, and K-ion batteries, thereby addressing the increasing demand for high-performance, renewable cathodes. The system integrates multiple predictive models to assess both the open-circuit voltage (VOC) and redox capacity of candidate molecules, enabling effective screening across extensive chemical spaces. Utilizing this system, they screened 45 million small molecules, ultimately identifying 3202, 689, and 702 redox-stable candidates for Li-, Na-, and K-ion batteries, respectively, thereby generating a targeted shortlist of high-potential materials for next-generation organic electrodes. The structure extends prior research that forecasted Li-ion insertion voltages by applying the approach to Na- and K-ion systems through a data-driven linear regression model (N-Linear Model, LM). The LM establishes a correlation between a molecule's reduction potential (PRed) and the battery's VOC. Model parameters are associated with the physical properties of alkali metals, such as electron affinity and Pauling electronegativity, which affect voltage trends. This enables the model to identify essential chemical relationships that influence electrochemical performance in various alkali-ion systems. The organic molecules for energy application database (OMEAD) was further expanded from 26,218 to 41,800 molecules, integrating features obtained from DFT calculations. A reduction potential neural model (RPNM) utilizes SMILES visualizations and natural language understanding to predict molecular decreased potentials. The LM uses these predictions to calculate the VOC, thereby creating a computational pipeline that eliminates the need for experimental observations or resource-intensive quantum calculations (Fig. 9f). The results also revealed that the structure integrates an RSNM to ensure the stability of candidate molecules under operational battery conditions. Molecules undergo initial screening for redox stability through the RSNM, followed by PRed prediction through the RPNM, and conclude with VOC estimation via the LM. This showed that linear models for Na- and K-ion batteries accurately predicted voltages, with model parameters correlating with the electron affinities and electronegativities of the alkali metals (Fig. 9g, h). The results further showed that thousands of new redox-stable molecules were identified for Li-, Na-, and K-ion batteries after DFT screening, with several candidates exhibiting promising voltages and multiple active redox sites, indicating potential for high energy density (Fig. 9i). Their work showed that this integrated AI-driven workflow enables rapid in silico evaluation of millions of organic molecules by combining stability assessment with voltage prediction. This structure integrates predictive accuracy with higher-throughput capability, serving as an effective tool for the accelerated rational design of next-generation, redox-stable organic cathodes for Li-, Na-, and K-ion batteries.

4.4. *Predictive modeling of charge, discharge, and degradation*

Understanding the charging–discharging behavior and degradation processes in energy storage devices is important for improving performance, safety, and longevity. These reactions entail intricate electrochemical, mechanical, and thermal relationships that standard modeling methods struggle to accurately represent [94]. ML and AI offer data-driven structures for predicting dynamic behaviors, including voltage profiles, internal resistance evolution, and capacity fade under different conditions. Predictive models that leverage extensive datasets can forecast cycle life, identify early indicators of degradation, and inform real-time control techniques for batteries and supercapacitors [95]. These methodologies are facilitating the development of advanced, self-optimizing energy storage devices with improved reliability and performance. For example, Lin et al. [96] proposed an approach for the early prediction of lithium-ion battery degradation across various charging strategies. The strategy integrates degradation behavior recognition with physics-guided modeling, acknowledging the limitations of real-world battery data and the challenges associated with long-term performance predictions. Essential steps include extracting optimal charging segments, clustering to identify typical degradation modes, enhancing limited data using polynomial fitting and Monte Carlo simulation, and implementing a transfer-learning structure that accounts for physical limitations. The approach effectively predicts degradation trajectories for 124 batteries, resulting in minimal errors (RMAE 0.0031 Ah, MAPE 0.215%), thus presenting a valuable tool for battery health management. The structure comprises four primary stages: feature extraction, degradation pattern identification, data augmentation, and model training utilizing transfer learning. Indicators of early-stage battery cycles are derived using a sliding-window methodology. K-means clustering reveals three distinct degradation types. Data augmentation employs polynomial fitting and Monte Carlo simulation on three reference batteries to produce simulated degradation data. Transfer learning leverages knowledge from reference batteries to inform target batteries, incorporating the physical constraints of convexity and monotonicity into the loss function to enable precise early-stage predictions of degradation trajectories. Four variants of the CNN-LSTM-Attention-TL network were further evaluated to determine the influence of physical limitations on battery degradation prediction: no constraints (W/OL1 + L2), convexity only (W-L1), monotonicity only (W-L2), and both convexity and monotonicity (W-L1 + L2, the proposed model). The analysis of 124 batteries indicates that including physical constraints improves prediction precision, with monotonicity having a greater impact than convexity. The W-L1 + L2 model demonstrates superior performance compared to alternative models, achieving reductions of 0.0018 Ah in average MAE, 0.0028 Ah in RMSE, and 0.191% in MAPE. This indicates that incorporating physical constraints improves the model's ability to represent degradation trends accurately (Fig. 10a). The results further showed that a fourth-order polynomial provides the best balance between accuracy and computational cost, significantly improving performance over third order while offering

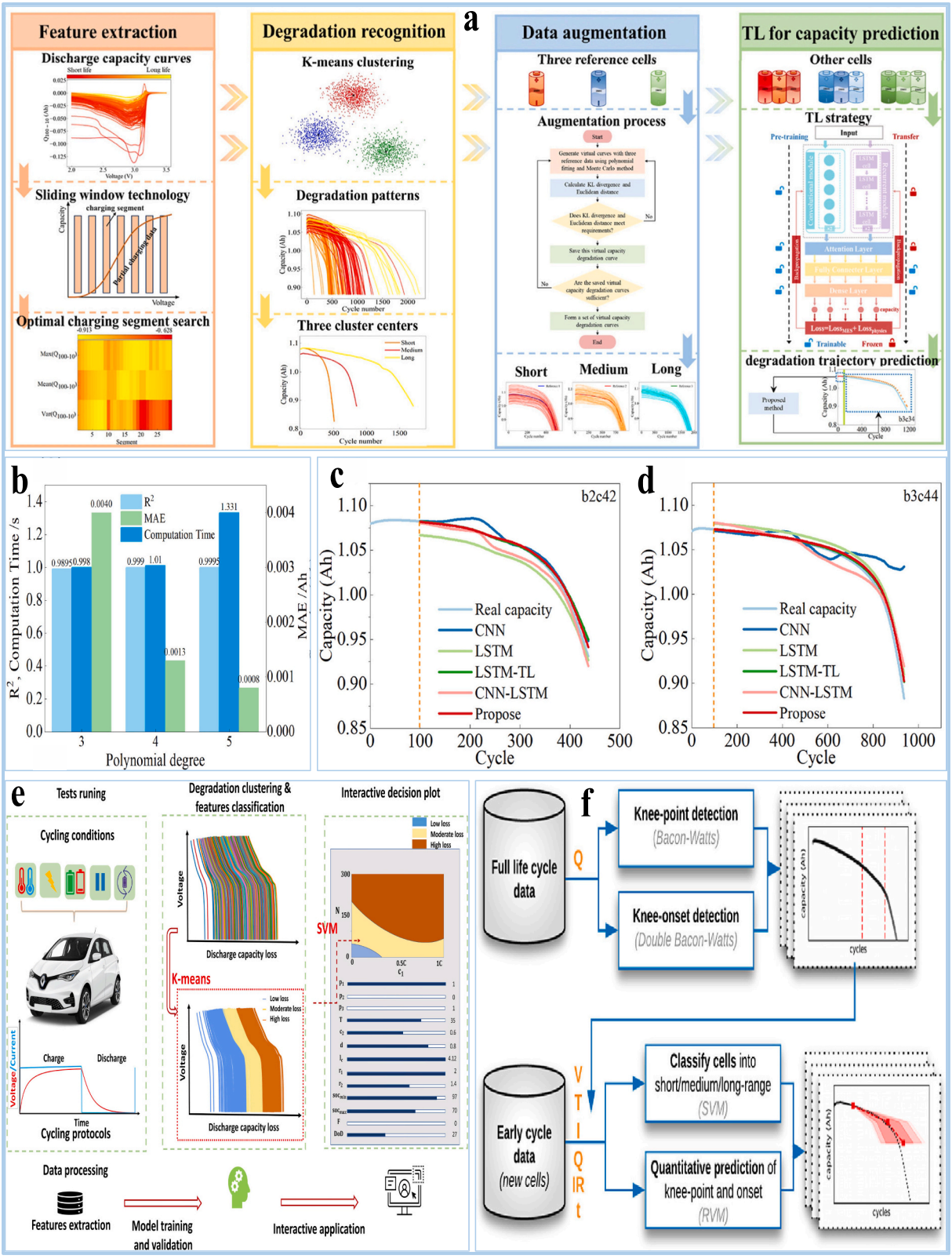


Fig. 10. (a) The suggested battery capacity deterioration trajectory prediction system; (b) R^2, MAE, and computation time of the model under different polynomial degrees; (c, d) Early battery degradation trajectory prediction results [96]. Copyright © 2025, Elsevier. (e) ML-based evaluation of operating conditions and process on industrial LiB cell degradation [97]. Copyright © 2025, Elsevier. (f) Schematic of ML prediction of knee-point and knee-onset in lithium-ion cell capacity degradation curves [98]. Copyright © 2020, Elsevier.

similar accuracy to fifth order with lower runtime (Fig. 10b). The results further showed that the proposed model outperformed CNN, LSTM, LSTM-TL, and CNN-LSTM in predicting battery degradation trajectories, achieving the closest match to actual capacity curves. It delivered the lowest prediction errors across 124 cells, with significant improvements in MAE, RMSE, and MAPE compared to all benchmarks. Incorporating the DP identification strategy further enhanced the accuracy of all models (Fig. 10c, d). Their study introduces a transfer learning framework that integrates pattern recognition, data augmentation, and physical constraints to facilitate early prediction of lithium-ion battery degradation.

Similarly, Malki et al. [97] designed an ML tool to analyze lithium-ion battery degradation in real automotive environments. Their ML model, intended for incorporation into battery management systems, categorizes aging conditions and protocols based on capacity loss. The model, developed using industrial datasets that incorporate various stress factors and characteristic interactions, demonstrates enhanced interpretability. An interactive application was developed to facilitate real-time exploration of parameter impacts, thereby supporting informed decisions to mitigate battery degradation. This research employs a systematic ML methodology, integrating k-means clustering and support vector machines, to categorize operating conditions and protocols in relation to lithium-ion battery capacity degradation. The strength of this approach lies in meticulous feature selection and a robust industrial dataset that spans a range of degradation rates and operating conditions. High-quality real-world data enhances the model's ability to identify hidden patterns and achieve reliable, precise classification. The findings from the random forest investigation indicate that all stress factors affect battery degradation to varying degrees, with differences observed across cell chemistries. Incorporating less significant factors improves the model's generalizability and transferability. Random forest rankings demonstrate predictive relevance, and correlation analyses uncover pairwise interactions, thereby reinforcing substantial insights and facilitating comparisons with existing literature (Fig. 10e). Their study introduces a tool that employs interpretable k-means and SVM models to investigate the impact of cycling and storage stress factors on LiB cell degradation, highlighting the importance of careful feature selection and balanced real-world data rather than relying on complex algorithms. Furthermore, Cueto et al. [98] formulated a comprehensive method for identifying and predicting critical points in lithium-ion battery capacity degradation curves, notably the "knee-onset," indicating the commencement of nonlinear degradation, and the "knee-point," where degradation significantly accelerates toward End-of-Life. Using capacity data from initial cycles, the ML models can accurately estimate these points with an average error of 9.4% based on only the first 50 cycles. The models define the expected cycle life of cells as short, medium, or long, with an accuracy of 88–90%, using data from only the first 3–5 cycles. This approach substantially reduces the time required compared to traditional End-of-Life prediction methods, which typically necessitate around 100 cycles. This strategy includes confidence metrics and prediction intervals, enabling manufacturers and energy storage operators to evaluate risk and guide warranty decisions. This approach serves as an effective tool for optimizing battery management, improving application-specific performance, and expediting validation of new cell production processes. Their study further examines the significant challenges of measuring uncertainty in ML predictions of lithium-ion battery degradation. The SVM model has been modified to classify expected cycle life into short, medium, and long categories, providing probabilistic outputs for each class. This adjustment enables the decision-making process to account for the relative costs of misclassification. They utilized conformal prediction intervals to determine model uncertainty in the quantitative prediction of knee-onset and knee-point. The intervals can be adjusted to encompass the true values with a specified probability, facilitating flexible trade-offs between confidence and precision. Regular cycle interval predictions facilitated effective experimental control by concentrating testing on cells with excessively broad prediction intervals, thereby optimizing laboratory resources use and increasing the accuracy of early-stage battery degradation forecasts (Fig. 10f). Their research demonstrated that early-cycle data can effectively predict battery lifetime, with the knee-point serving as a more significant metric than total cycle life for enhancing usage, production, fast-charging strategies, and battery insurance. In addition, across energy storage systems, battery-focused ML studies predominantly rely on time-series electrochemical data to predict degradation, lifetime, and safety. In contrast, supercapacitor research emphasizes structure–property relationships using material descriptors such as surface area and porosity, as summarized in Table 2, which highlights the differences in material systems, algorithms, datasets, and target performance metrics across these technologies. Additionally, hybrid systems such as MXenes and MOFs underscore the growing importance of multimodal datasets, which combine structural, electrochemical, and physicochemical inputs for more comprehensive modeling. This comparison clearly indicates that ML models in batteries are primarily prediction-driven, focusing on performance forecasting and reliability, while supercapacitor studies are more design-oriented, emphasizing material optimization and enhanced electrochemical properties.

5. Integrated and cross-cutting applications

The advancement of energy and electronic technologies is driving the convergence of light-harvesting, energy-conversion, and storage devices. The upcoming generation of renewable devices is designed to successfully capture and store energy while integrating multiple functionalities into a unified structure [99]. Reaching this integration necessitates an in-depth knowledge of complex, interrelated physical processes, namely electronic, optical, thermal, and electrochemical, that conventional design methodologies find challenging for optimizing concurrently [100]. ML and AI are increasingly integral in connecting these domains. The development of multifunctional materials and devices is facilitated, inverse design procedures for targeted property optimization are accelerated, and multiphysics simulations that demonstrate the interaction among optical, electronic, and electrochemical processes are enhanced [101]. Photo-rechargeable batteries, self-charging supercapacitors, and hybrid optoelectronic systems represent advancements in energy technology. Data-driven methodologies are enabling the development of intelligent, adaptive devices that can efficiently harvest and store energy [102]. This section examines the various cross-cutting developments, concentrating on (i) integrated optoelectronic–energy storage mechanisms, (ii) ML-enabled development of multifunctional devices, (iii) inverse design and generative modeling for novel materials, (iv) AI-enhanced multi-physics simulations, and (v) AI-assisted TENG–supercapacitor hybrid systems based on MXene–MOF–chalcogenide architectures that integrate development and discovery across multiple disciplines.

5.1. Coupled optoelectronic-energy storage devices

The integration of energy harvesting and storage into a unified platform represents a significant advancement in the development of autonomous, sustainable power devices. Coupled optoelectronic-energy storage devices, including photo-rechargeable batteries, self-charging supercapacitors, and solar capacitors, integrate photovoltaic and electrochemical properties into a single structure [103]. These devices capture solar energy and store it directly, eliminating the need for separate conversion units and minimizing overall energy loss [104,105]. The primary challenge is to achieve effective coupling among photon absorption, charge separation, and ion transport processes, which are often influenced by competing kinetics and interfacial limitations [106]. ML and AI are advancing in this field by enabling the formation of multifunctional materials, improving device performance, and predicting efficiency under realistic operating conditions. Data-driven models

Table 2
Comparative summary of ML applications in energy storage systems.

Systems	Device type	ML/AI algorithm	Input features	Target metrics	Main efficiency	Key insight	Ref.
Li-ion	Battery	ANN, RF	Cycling data	Capacity, SOH	>95%	Degradation prediction	[77]
Solid-state	Battery	SVM	Conductivity	Stability	Fast discovery	Safer design	[78]
Na-ion	Battery	GB	Descriptors	Capacity	Efficient	Alt to Li	[79]
MXene	Supercapacitor	DL	Surface features	Capacitance	High accuracy	Correlation	[85]
Carbon	Supercapacitor	RF	Porosity	Capacitance	Optimized	Screening	[86]
Fe-SnO_2/MXene	Supercapacitor	ML	Electrochem	Capacitance	1225.6 F/g	Hybrid effect	[87]
Redox flow	Battery	Regression	Electrolyte	Efficiency	Improved	Scalable	[91]
MOF	Hybrid	DL	Structure	Energy density	Enhanced	Multifunction	[97]

facilitate the analysis of intricate relationships among optical and electrochemical parameters, thereby supporting the design of materials that demonstrate robust light absorption, high conductivity, and reliable storage capacity [107]. AI-assisted techniques are transforming the synthesis of next-generation self-powered structures that enable continuous, intelligent energy harvesting and storage for flexible electronics, sensors, and portable devices [108]. For example, Gu et al. [109] investigated integrating ML with self-charging power sources (SCPS), emphasizing the combination of triboelectric nanogenerators (TENGs) and modern energy storage technologies to develop effective, versatile, and feasible power solutions. TENGs have garnered considerable interest due to their ability to harvest various ambient mechanical energy sources, including human motion, vibrations, and environmental motion. Their substantial energy output, affordability, and environmental friendliness make them suitable candidates for next-generation self-powered devices. Nonetheless, since TENGs produce alternating current (AC), it is necessary to rectify and manage the energy using appropriate circuitry before storage in an energy device, thereby ensuring efficient conversion and utilization. They suggested a self-charging power system that integrates TENGs with SC, which exhibit increased power density, accelerated charging/discharging rates, and enhanced cycling stability relative to traditional batteries. This integration enables concurrent energy harvesting, transformation, and storage, resulting in a compact, effective power unit that provides continuous energy for mobile and wearable devices. They further identified the constraints of conventional solid self-charging devices and subsequently progressed the field by developing adaptable fiber-like self-charging structures capable of seamless integration with textiles

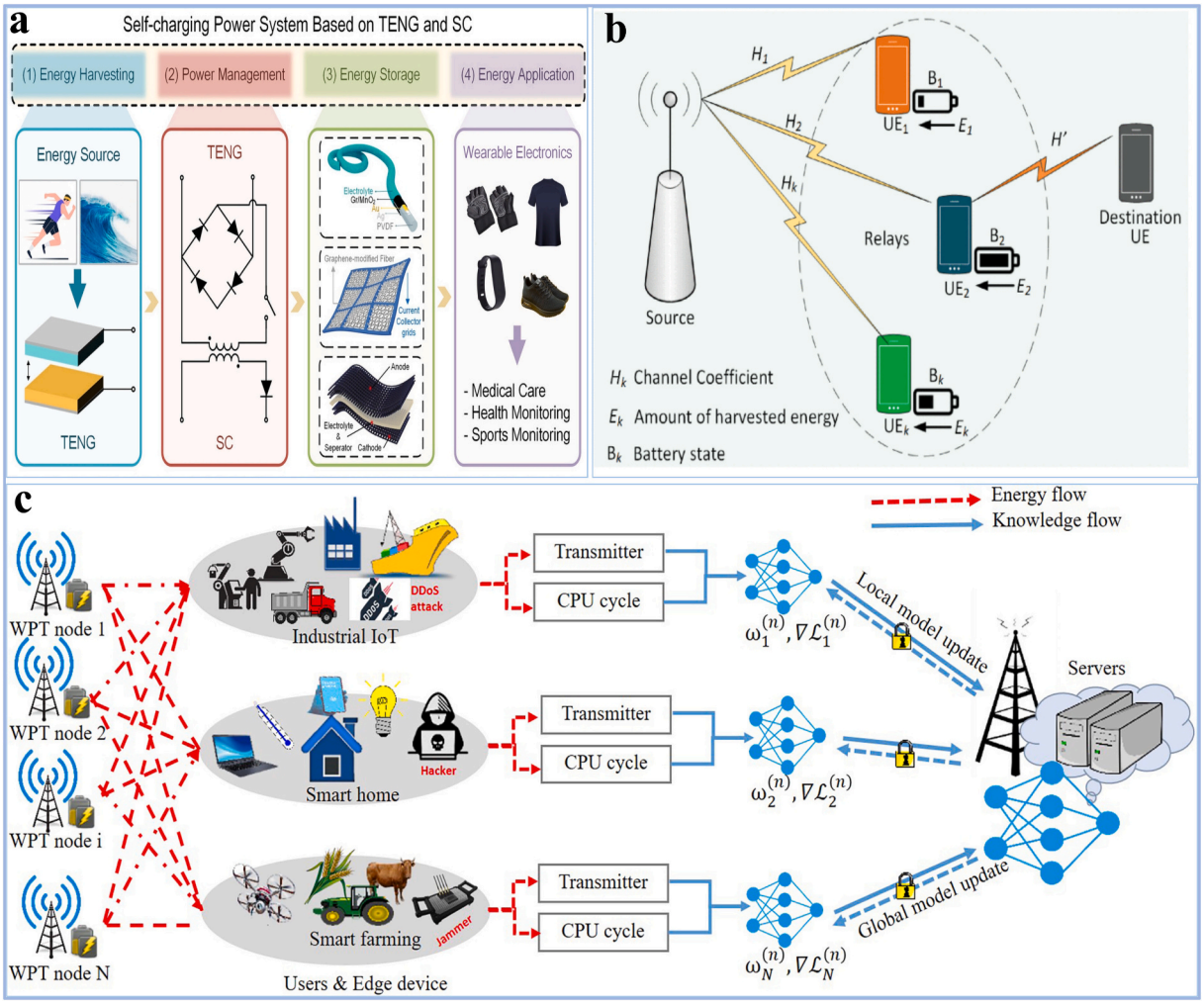


Fig. 11. (a) Schematic illustration of a self-charging power system using TENG and SC [109] Copyright © 2025, John Wiley and Sons. (b) A collaborative EH IoT networking [114] Copyright © 2025, IEEExplore. (c) A scenario for using AI to improve EH reliability [115] Copyright © 2023, Elsevier.

and wearable devices. Their coaxial fiber network features a one-dimensional design that integrates an external TENG and an internal SC within a single structure. The outer TENG layer captures mechanical energy from motion or environmental sources, whereas the inner SC effectively stores the transformed energy. The structure employs carbon fibers as electrodes and silicone rubber as a separator and triboelectric layer, demonstrating notable flexibility, reliability, and energy stability, even under repeated mechanical stretching. Their study further showed the multifunctionality of these mechanisms, which provide reliable power for small devices, including wristwatches and thermometers, and also serve as self-powered tactile and pressure sensors. The fiber-based design demonstrates notable performance metrics, including elevated output power, substantial capacitance, and exceptional sensitivity, rendering it appropriate for real-time monitoring and intelligent sensing in wearable electronics. They also improved the predictive and optimized abilities of their SCPS design through the integration of ML algorithms. ML models were used to assess energy conversion performance, forecast degradation, and improve materials and designs for enhanced output. This data-driven methodology enables effective energy management, adaptive control, and increased system dependability (Fig. 11a). Their work represents a thorough and insightful approach to developing ML-assisted, flexible self-charging power systems. This strategy integrates energy harvesting, storage, and real-time system performance, facilitating the development of next-generation self-sustaining, wearable, and multifunctional electronic devices. Similarly, Raza et al. [110] proposed an autonomous hybrid electric vehicle system that integrates AI and the Internet of Things (IoT), featuring a self-charging facility to address significant challenges in energy conservation and charging. The study emphasizes that integrating AI and IoT enables real-time monitoring of charging efficiency, data exchange between vehicles and their environments, and sensor-based regulation for autonomous driving. The AI system improves decision-making, energy management, and automation, facilitating the emergence of self-charging electric vehicles that minimize charging time, alleviate parking challenges, and reduce traffic congestion, while also advancing smart city infrastructure. The research indicates that IoT serves as a fundamental technology in contemporary intelligent transportation, facilitating seamless connectivity among diverse vehicle components, external sensors, and cloud-based systems. IoT integration enables vehicles to monitor and control various parameters in real time, facilitating the transmission of vital data to operators or other vehicles through the internet. Hybrid and autonomous vehicles utilize IoT systems that integrate data from cameras, onboard sensors, smartphones, traffic monitors, and parking detectors to optimize operational performance and enhance safety. These devices use cloud computing to enable vehicles to analyze large volumes of data for real-time traffic management, route optimization, and predictive maintenance. The integration of AI with IoT enables autonomous vehicle operation across diverse driving and environmental conditions. The integration of these technologies facilitates informed decision-making, prompt fault identification, and immediate notifications in the event of irregularities. AI and IoT are revolutionizing the automotive industry by enabling the creation of autonomous, self-monitoring, and energy-efficient vehicles, representing a vital advancement toward fully integrated, intelligent mobility systems. Their research demonstrated that integrating IoT enables real-time monitoring and autonomous control, thereby enhancing safety, productivity, and connectivity in contemporary vehicles.

5.2. ML for multifunctional device design

Multifunctional energy devices are designed to integrate various processes, including light harvesting, transformation, and electrochemical storage, into a unified and coordinated structure. Developing integrated systems necessitates the optimization of various physical, chemical, and structural parameters that interact nonlinearly, posing a considerable challenge for traditional experimental or simulation-based design approaches [111]. ML offers a solution by facilitating data-driven exploration across intricate design spaces, uncovering hidden correlations that influence multifunctional efficiency. Using supervised and reinforcement learning methods, ML models can predict the impact of variations in material formulation, morphology, or structure on energy transformation efficiency and storage [112]. This potential enables researchers to discover synergistic combinations of materials, improve surface engineering, and design innovative hybrid structures, including photo-supercapacitors and piezo-photocatalytic systems. As ML evolves, it enables the automation and enhancement of the development of highly effective, adaptive devices capable of simultaneously harvesting, storing, and managing energy in real time [113]. For example, Alamu et al. [114] conducted a detailed investigation of reinforcement learning (RL) in energy-harvesting (EH) IoT networking, highlighting the potential of RL methods to enhance decision-making in dynamic, uncertain conditions. Several reinforcement learning techniques suitable for the EH IoT were highlighted, such as multi-armed bandits (MAB), Markov decision processes (MDP), dynamic programming, and temporal difference learning. Each approach provides methods for maximizing cumulative rewards through learning from environmental conversations. These approaches are essential in EH IoT networking, where nodes must adaptively decide under constraints of limited energy and fluctuating network conditions. Their work primarily centered on the MAB method, enabling IoT nodes to make sequential decisions that balance investigation-examining lesser-known actions to uncover potential high rewards, and exploitation-selecting the best-known actions to optimize immediate returns. Each action generates a reward according to an unspecified probability distribution, and over time, the node acquires knowledge of which actions provide the greatest advantage. The MAB technique effectively minimizes cumulative regret and guarantees optimal long-term network performance by strategically balancing exploration and exploitation, even under conditions of uncertainty or incomplete information. They further addressed a relay selection problem in EH IoT networks, focusing on maximizing throughput to illustrate the practical application of MAB. In this scenario, a single source node transmits data to a destination device through several EH IoT nodes functioning as relays. Each relay functions as an “arm” within the MAB framework, with the source selecting a relay in each time slot according to its anticipated reward, measured by the signal-to-interference-plus-noise ratio (SINR). Continuous monitoring and updating of the expected rewards for each relay enables the source to implement an optimal selection policy, thereby maximizing throughput and preventing data outages and network mistakes (Fig. 11b). Their study illustrates that reinforcement learning, specifically the MAB approach, offers a strong and adaptable structure for decision-making in EH IoT networking. These methods enhance network reliability, energy efficiency, and overall system performance by enabling nodes to learn from interactions, improve relay selection, and adapt to dynamic environmental conditions, thereby facilitating the development of more intelligent and autonomous IoT-enabled energy-harvesting systems. Similarly, Masoumeh et al. [115] emphasized that EH serves as a vital power source for IoT networking, enabling the autonomous and sustainable operation of low-power devices. EH systems are susceptible to security threats, including eavesdropping, data manipulation, and denial-of-service attacks, potentially leading to the leakage of sensitive data and a reduction in harvested energy. Their study showed that EH can be achieved using both RF (radio frequency) and non-RF sources, each with distinct advantages. RF energy harvesting involves collecting electromagnetic radiation from various sources, including Wi-Fi, cellular networks, radio and television broadcasts, and RFID tags. This enables power delivery to devices situated in remote or difficult-to-reach areas; however, the EH is typically constrained, rendering it most appropriate for lower-power applications such as sensors and fragile wireless devices. Non-RF EH gathers energy from various environmental sources such as light, heat, vibrations, and mechanical motion, thereby offering a wider and more stable energy input. The integration of RF and

non-RF methods facilitates a continuous consistent power supply, thereby ensuring the uninterrupted operation of IoT and other lower-power systems. Furthermore, the study demonstrated that wireless power transmission (WPT) can enhance energy harvesting by providing energy without the need for physical connections. WPT technologies, including inductive coupling, magnetic resonance, electromagnetic waves, and laser power beaming, facilitate effective power delivery to devices situated in remote or difficult-to-access locations, thereby eliminating the constraints and inconveniences associated with wired connections. WPT presents several challenges, including limited transmission range, performance degradation, and the potential for interference with adjacent electronic devices. Their research aims to enhance the productivity, range, and reliability of WPT, establishing it as a viable technology to complement both RF and non-RF energy harvesting methods (Fig. 11c). Their research showed that the integration of RF and non-RF energy harvesting, WPT, and AI-enhanced security establishes a comprehensive structure for the power supply and protection of IoT networking. This structure ensures the effective, continuous, and secure operation of contemporary low-power devices in dynamic, distributed environments.

5.3. Inverse design and generative materials modeling

Conventional methods for materials discovery typically utilize forward approaches, which involve testing well-known materials and simulating their properties to identify optimal candidates. Inverse design, in contrast, reverses the traditional approach by starting with a desired property or performance and using computational methods to determine the necessary structure or composition to realize it [116]. Generative models, including variational autoencoders (VAEs) [117], generative adversarial networks (GANs) [118], and diffusion models [119], have been developed as effective tools for implementing this idea in materials science. By analyzing extensive datasets comprising established materials, these models can produce innovative compositions and crystal structures that meet defined parameters, including elevated ionic conductivity, optical absorption, or mechanical stability. Inverse engineering has been utilized in energy-related disciplines to identify new electrode materials, solid electrolytes, and light-absorbing semiconductors that exhibit enhanced performance [120]. The integration of generative models with DFT calculations and experimental feedback loops facilitates the development of closed-loop discovery structures that consistently enhance and suggest improved candidates. This combination represents a significant advancement in AI-powered autonomous materials design, effectively shortening discovery timelines from years to weeks [121]. For example, Lee et al. [122] investigated ML-based inverse design techniques for materials, highlighting the effect of data features and design space size on design performance and precision. They demonstrated that inverse design problems can be categorized into four distinct cases. In small design spaces with extensive datasets, conventional interpolation-based ML techniques are adequate. In extensive design spaces, methodologies such as active learning or meticulously crafted DNNs are essential for tackling weak generalization beyond the training dataset. Transfer learning and multi-fidelity regression may improve predictions when simulations and experiments, or lower- and higher-fidelity datasets, differ. In constrained design environments characterized by limited datasets, Bayes's algorithm effectively determines optimal solutions while minimizing data collection efforts (Fig. 12a). They demonstrated that inverse modeling network can efficiently predict design variables based on desired material performance. Conventional DNNs exhibit limitations in handling one-to-many mappings, where various designs can produce equivalent performance outcomes. They further addressed this issue by grouping training data to eliminate duplicate efficiency, training distinct inverse networking for each group, and integrating them into a unified prediction model, which markedly enhanced accuracy relative to traditional DNNs. These studies collectively illustrate methods to improve prediction accuracy, generalization, and productivity in materials design utilizing ML. Similarly, Wang et al. [123] investigated the inverse design of materials through ML, a methodology that fundamentally contrasts with conventional direct development methods. The direct design approach starts from a defined chemical composition or molecular structure to forecast the resultant material properties. Inverse design, by contrast, begins with specified target properties or desired functionalities and systematically deduces the molecular structures or chemical compositions necessary to realize them. This method enables researchers to systematically explore chemical space, focusing on identifying configurations that satisfy defined efficiency criteria rather than evaluating arbitrary combinations. Prioritizing target performance in inverse design facilitates a goal-oriented investigation of molecular or materials space, thereby enhancing the performance of the design approach. The authors further emphasized that inverse design poses significant computational challenges owing to the vast, high-dimensional search space and the problem's ill-posedness. Multiple distinct materials often fulfill the same target property, resulting in ambiguity and complexity in optimization. A range of strategies has been implemented to tackle these challenges. Genetic algorithms and adjoint methods systematically explore the search space, whereas Bayesian structures, low-dimensional estimations, and annealing techniques facilitate complexity management and improve integration with optimal solutions. They also highlighted three primary modalities of inverse engineering: first, searching for artificial superstructures that fulfill target functionality; second, exploring the chemical ingredient space; and third, identifying missing or unreported compounds that satisfy the specified efficiency criteria. Modern methods, including high-throughput virtual screening, global evaluation, and generative models, are frequently employed to navigate this chemical space effectively. High-throughput screening enables rapid assessment of numerous candidate materials, while global optimization ensures convergence to optimal solutions in complex landscapes. Additionally, generative models can suggest novel material structures based on specified properties (Fig. 12b). Their work showed that these methods illustrate that ML-based inverse design offers a systematic, effective, and adaptable structure for materials discovery, allowing researchers to focus on specific functionalities in the design process. Similarly, Fuhr et al. [124] examined inverse design and generative models (GMs) for innovative materials, emphasizing a significant challenge: selecting the structure representation or descriptors. Simplified descriptors, including composition and select physical properties, demonstrate robustness and generalizability across extensive material databases; however, their predictive power is limited, especially concerning phenomena such as polymorphism. Conversely, intricate descriptors that capture detailed atomic structures enhance model specificity and accuracy; however, they also increase the risk of overfitting, require greater memory, and diminish the model's capacity to generalize beyond a limited range of materials. The trade-off between simplicity and specificity is vital in the development of efficient generative models for materials discovery. They further indicated that material structures can be displayed in three primary forms for generative modeling: (1) phase-fields, which denote elemental combinations that indicate distinct chemistries; (2) composition, which specifies particular atomic structures; and (3) coordinate or image-based structures, which capture detailed aspects such as lattice parameters or atomic coordinates. Every representation entails trade-offs regarding complexity and predictive capability. The selection of a suitable generative model structure, such as GANs or VAEs, is essential for material generation, as various structures are tailored to specific types of structural representations (Fig. 12c). They demonstrated that deep-learning pipelines utilizing VAEs or GANs acquire visualizations of material data distributions and produce new samples through the exploration and manipulation of a latent space. In VAEs, an encoder network transforms high-dimensional data, such as a material structure, phase-field, or mixture, into a low-dimensional latent space. Subsequently, a decoder network maps the latent representation back to

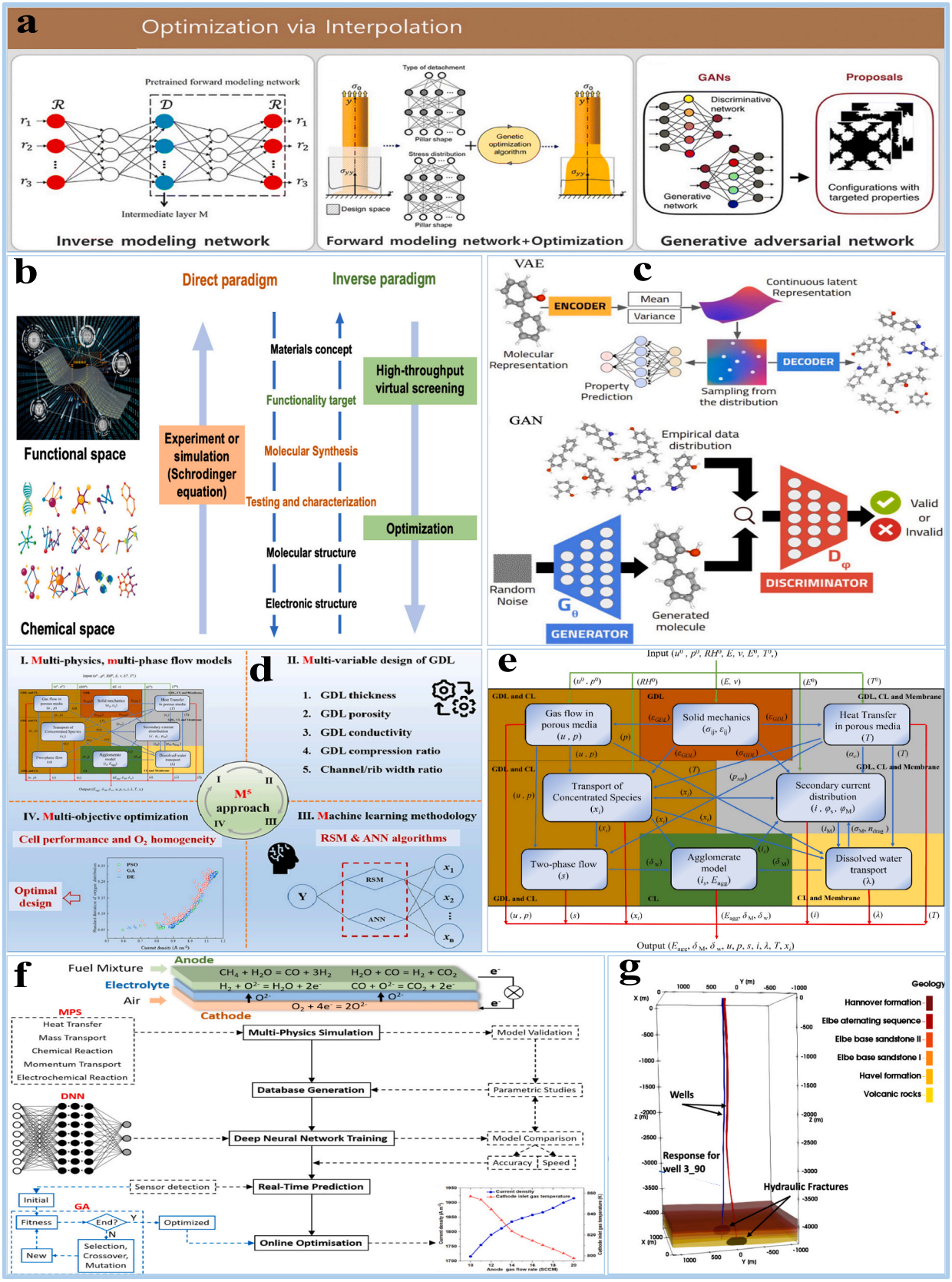


Fig. 12. (a) Illustration of a scenario with abundant data and a relatively limited design space [122] Copyright © 2023, Royal Society of Chemistry. (b) Schematic overview of different strategies for molecular design [123] Copyright © 2022, MDPI. (c) Commonly employed generative model architectures for molecular generation [124] Copyright © 2022, Frontiersin.org. (d) Illustration of the PEMFC unit and its modeling domain; (e) Diagram of the computational workflow [130] Copyright © 2023, Elsevier. (f) Representation of an SOFC with a complex fuel mixture [131] Copyright © 2020, Elsevier. (g) Overview of the geothermal reservoir model at Groß Schönebeck [132] Copyright © 2022, Nature.

produce new material structures. The method estimates the posterior distribution of the data to generate new materials. Traditional autoencoders follow a similar encode-decode structure, focusing solely on reconstructing the original input and primarily functioning as a tool for pre- or post-processing in materials discovery. Variations in VAE and GAN structures demonstrate distinct approaches to learning and sampling from the data distribution.

5.4. AI-enhanced multi-physics simulations

Energy storage and optoelectronic systems operate through the interaction of various physical phenomena, including charge transport, photon absorption, ionic diffusion, heat transfer, and mechanical stress. Accurately simulating these relationships across multiple spatial and temporal scales remains a primary challenge in device engineering [125]. Conventional numerical models, while effective, often incur high computational costs and are constrained by assumptions that may oversimplify real-world conditions [126]. Multi-physics simulations improved by AI overcome these limitations by integrating physics-based modeling and data-driven learning methodologies. ML algorithms can approximate complex physical functions, reduce computation time, and enhance predictive accuracy through adaptive learning techniques [127]. Surrogate models trained on simulation or experimental data can quickly predict outcomes, including charge distribution, temperature characteristics, and degradation routes under different conditions [128]. Furthermore, hybrid AI-physics systems facilitate real-time co-simulation of electronic, optical, and thermal properties, thereby offering a comprehensive understanding of device behavior. Recent advancements are allowing researchers to design devices that are more effective, robust, and multifunctional, achieving a level of precision that accelerates innovation in integrated energy systems [129]. For example, Wang et al. [130] investigated integrating multi-physics simulations with ML-based surrogate modeling to conduct a multi-objective analysis of the distorted gas diffusion layer (GDL) in proton exchange membrane (PEM) fuel cells to improve performance and stability. They discovered that PEM fuel cells, an essential technology for achieving a low-carbon future, have experienced a significant acceleration in innovation driven by AI. The GDL significantly affects heat and water management; thus, maximizing factors such as thickness, porosity, conductivity, channel/rib size, and compression ratio is essential for enhancing performance. Their study compares response surface methodology (RSM) and ANNs, illustrating that the M5 model significantly improves GDL optimization. The customized design enhanced current density by 20.8% and decreased oxygen distribution variation by 74.6%, establishing a Pareto front to balance efficiency and homogeneity (Fig. 12d). Their physics-based model was further verified against experimental results, demonstrating substantial correlation between the generated and observed polarization structures, with an average deviation of merely 0.01 A cm^{-2} at 0.4 V. This validated the model's reliability in examining non-uniform gas diffusion layer deformation and its impact on transport dynamics and oxygen distribution. Predictive accuracy was assessed by comparing data-driven surrogate models, such as RSM and ANNs, with the physics-based model. The relationship between estimated and actual values was assessed through the R^2 and RMSE. The results indicated that all models attained excellent precision, exhibiting R^2 values of 0.828, 0.838, and 0.994 for RSM, ANN46, and ANN114, respectively, along with corresponding RMSEs of 0.010, 0.034, and 0.008. The ANN models exhibited enhanced data correlation recognition relative to RSM, with performance markedly improving as the size of the training dataset increased. The improved ANN114 model demonstrated strong predictive ability for oxygen distribution, achieving a R^2 of 0.993 and an RMSE of 0.004. This confirms that ANN-based surrogate models provide a reliable and effective method for enhancing PEM fuel cell development (Fig. 12e). Similarly, Xu et al. [131] investigated the combination of deep learning and multi-physics simulations to facilitate real-time enhancement of solid oxide fuel cell (SOFC) performance. Neural networks were used to efficiently predict system actions, boosting accuracy and processing performance over traditional simulations. Their research illustrated that integrating multi-physics simulation with deep learning offers an effective and efficient method for real-time evaluation and enhancement of SOFC. This hybrid structure successfully integrates the precision of physics-based modeling with the performance of AI-driven prediction. Training a DNN on simulation data resulted in a prediction error of less than 1% relative to MPS, while significantly decreasing the computational cost and time needed for optimization. The system utilized a genetic algorithm to optimize essential performance metrics, including power density, heat generation, and temperature gradients, thereby ensuring effective and stable operation of the SOFCs under dynamic conditions. This method improves the long-term performance and reliability of SOFCs while developing a structure applicable to the optimization of other complex, nonlinear energy systems in real time (Fig. 12f). Furthermore, Degen et al. [132] examined 3D multi-physics uncertainty quantification through a physics-based ML structure aimed at enhancing the accuracy and performance of predicted complex physical phenomena. Their approach integrated data-driven learning with physics-informed constraints, enabling accurate modeling of multi-physics systems under uncertainty. They demonstrated that quantitative predictions of Earth's subsurface require substantial computational resources because of the high-dimensional, interconnected physical equations involved. To address this issue, a hybrid physics-derived ML strategy, specifically the non-intrusive reduced basis (NI-RB) approach, was introduced to develop reliable, scalable, and interpretable surrogate models. This approach combines physical models with data-driven methodologies, enabling probabilistic analyses such as global sensitivity studies and uncertainty quantification while achieving significant computational speedups without sacrificing accuracy. The structure, while illustrated in the context of a thermo-hydro-mechanical reservoir, is applicable to a wide range of geoscientific issues (Fig. 12g). The NI-RB surrogate model was utilized in a real geothermal reservoir, which effectively captures high-dimensional, tightly coupled multi-physics phenomena. It effectively replicated complex pore-pressure evolution, encompassing both fast, short-term fluctuations and long-term trends that traditional deep learning models struggle to capture. The model attained a high level of accuracy using only five basis functions, with values of 2.29×10^{-7} for training and 2.48×10^{-4} for validation, surpassing the precision of the original finite element model. Their work indicates the performance of the NI-RB approach for conducting efficient, high-fidelity simulations of complex multi-physics systems.

5.5. AI-assisted TENG–supercapacitor hybrid systems based on MXene–MOF–chalcogenide architectures

The integration of energy harvesting and storage into cohesive platforms has become an essential approach for advancing self-sustaining electronic systems. Among these, triboelectric nanogenerator (TENG)-based hybrid systems integrated with supercapacitors constitute a promising class of devices that can simultaneously convert mechanical energy into electrical energy and store it for future use [133]. Recent studies have shown that MXene-based conductive structures [134,135], metal–organic frameworks (MOFs)-based porous structures [136,137], and transition metal chalcogenides (TMCs) [138,139] can be synergistically combined in TENG-supercapacitor systems, facilitating improved energy conversion and storage within a unified platform. These hybrid structures leverage the synergies between the two material classes, resulting in enhanced device performance and multifunctionality. MXenes, comprising two-dimensional transition-metal carbides and nitrides, exhibit high electrical conductivity, hydrophilic surfaces, and adjustable surface terminations, making them strong candidates for charge transfer and electrode synthesis in TENG-supercapacitor structures [140]. Their potential to create adaptable and conductive networks enhances effective electron transmission

and reduces internal resistance [141]. MOFs offer highly porous, structurally adaptable structures that facilitate ion transport and augment the electrochemically active surface area, thereby enhancing capacitance and charge storage performance [142,143]. Moreover, TMCs (e.g., MoS_2 and WS_2) exhibit significant electrochemical activity and layered architectures that facilitate fast redox reactions and additional charge storage. The combined effect of these materials produces a synergistic interface that improves both triboelectric output and electrochemical performance [144]. Notwithstanding these benefits, optimizing complicated hybrid systems remains difficult due to the extensive interconnections among mechanical energy harvesting, charge transport, and electrochemical storage mechanisms. In this context, ML methods have emerged as potent tools for improving predictive performance in energy conversion efficiency, charge storage properties, and long-term stability in TENG–supercapacitor networks [145]. Data-driven models may evaluate complex interactions among material composition, structural factors, and device architecture, therefore determining optimal design structures that are challenging to attain via traditional trial-and-error methods [146]. ML-assisted structures enable the prediction of key performance metrics, such as triboelectric output voltage, capacitance, energy density, and cycling stability, across diverse operational conditions. Methods such as supervised learning, reinforcement learning, and surrogate modeling enable rapid evaluation of material combinations and device designs, thereby

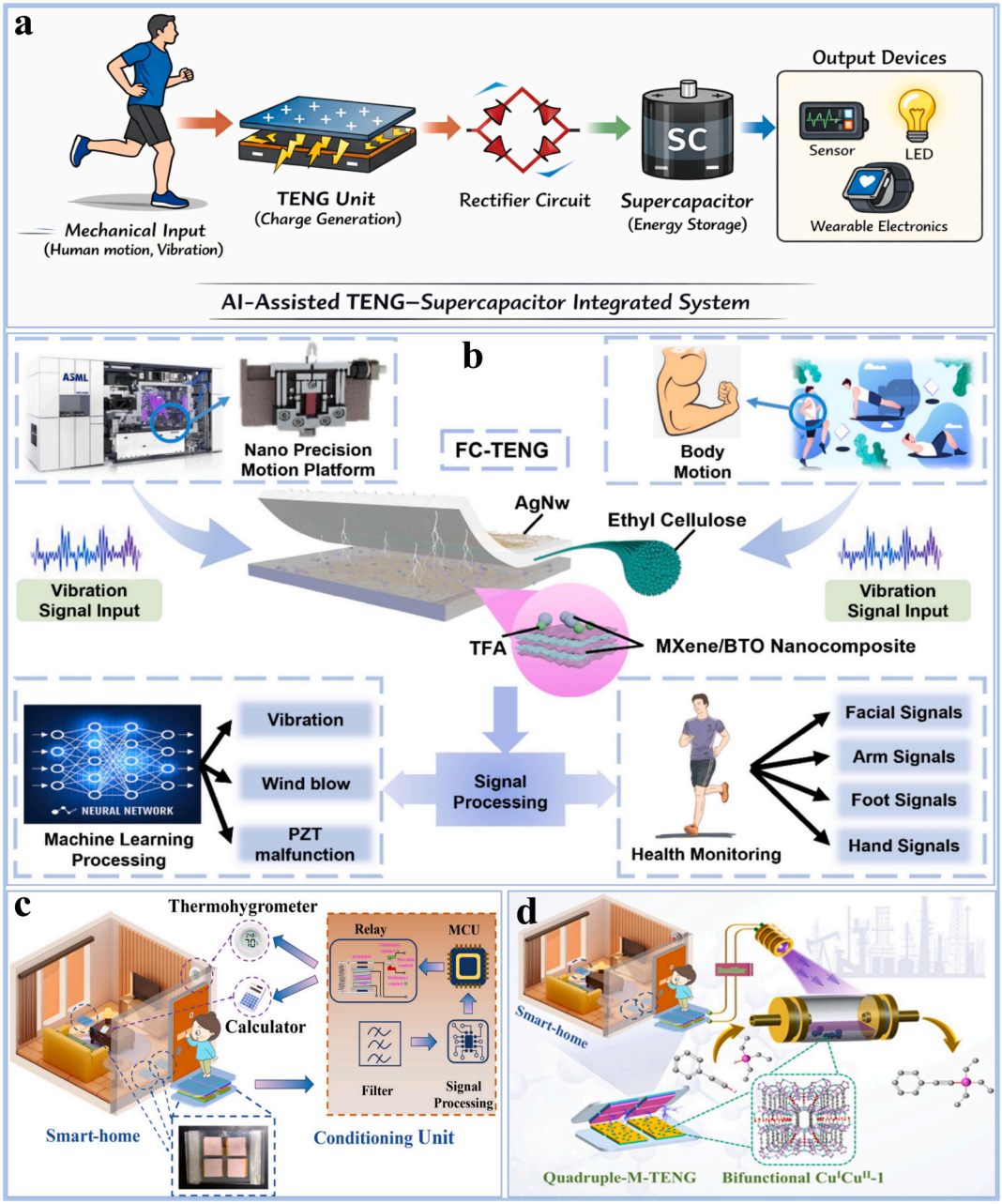


Fig. 13. (a) Schematic of an AI-assisted TENG–supercapacitor integrated system based on MXene–MOF–chalcogenide architectures, where mechanical energy is converted by a TENG, rectified, stored in a supercapacitor, and used to power electronic devices, with ML enabling performance optimization. (b) Flexible MXene/$BaTiO_3$-based TENG with ferroelectric coupling for enhanced pressure sensing, self-powered operation, and real-time intelligent health monitoring via deep learning-assisted signal recognition [151] Copyright © 2025, Elsevier. (c) ML-assisted design of bifunctional MOF-based TENG systems for integrated energy harvesting and self-powered photocatalysis; (d) Schematic illustration of controlling smart home appliances using quadruple-M-TENG-based smart boards [152] Copyright © 2024, American Chemical Society.

markedly expediting the design process [147]. Moreover, AI-driven optimization can address significant issues, including impedance matching between TENG and supercapacitor units, charge rectification performance, and interfacial energy losses. Those attributes are vital for attaining effective energy transfer and optimizing overall system performance [148]. Furthermore, integrating AI into experimental workflows enables the formation of closed-loop optimization systems, in which model predictions are continually refined through real-time feedback from device performance. This methodology facilitates the systematic design of advanced self-powered systems that integrate MXene–MOF–chalcogenide hybrid materials with sophisticated control mechanisms, hence enabling the development of adaptive, high-efficiency energy devices [149]. These systems are especially advantageous for wearable devices, IoT sensors, and portable energy platforms, where a constant, reliable power supply is essential [150].

For example, Fig. 13a presents a schematic representation of an AI-assisted TENG-SC integrated system based on the energy nexus concept. Similar to previous developments in MXene–MOF–chalcogenide hybrid structures, mechanical energy inputs, including human movement or ambient vibrations, are initially converted into electrical impulses by the TENG unit. The produced alternating current is subsequently rectified by a power management circuit to yield a stable direct current. This electrical energy is then stored in a supercapacitor, enabling efficient charge accumulation and rapid energy delivery. The accumulated energy powers small electronic devices, including sensors, LEDs, and wearable technology. ML and AI structures can be incorporated into this system to enhance material selection, device design, and energy management, thereby facilitating predictive control of charge generation, storage efficiency, and long-term operational stability. Similarly, Yuan et al. [151] presented a flexible ferroelectric-coupled MXene/$BaTiO_3$-based TENG designed for improved pressure sensing and advanced health monitoring applications. The device was synthesized by integrating MXene nanosheets and $BaTiO_3$ nanoparticles into a flexible styrene-ethylene-butylene-styrene (SEBS) polymer matrix, yielding a composite with enhanced dielectric and ferroelectric properties. The use of $BaTiO_3$ facilitated robust ferroelectric polarization, whereas MXene enhanced electrical conductivity and surface charge transfer, resulting in an elevated dielectric constant and diminished energy dissipation. The ferroelectric coupling significantly enhanced charge trapping and release, thereby improving the TENG's output voltage, current, and overall sensitivity. The device demonstrated an extensive linear response range and superior mechanical flexibility, rendering it appropriate for wearable and real-time sensing applications. It proved proficient at precisely detecting diverse human motions and physiological signs, including finger tapping, joint movement, and small pressure fluctuations (Fig. 13b). Moreover, integrating the TENG with a sophisticated deep learning system featuring an attention mechanism enabled accurate, instantaneous classification of pressure signals. This integration of high-performance energy harvesting, precise pressure sensing, and advanced data processing demonstrates the system's significant potential as a self-sustaining, adaptable platform for next-generation human-machine interfaces and intelligent health-monitoring devices. Furthermore, Zhang et al. [152] presented an ML–informed approach to creating bifunctional MOFs that concurrently improve TENG and photocatalytic efficiencies for self-sustaining systems. They synthesized two MOFs, one of which is a mixed-valence Cu(I)/Cu(II) structure (CuICuII-1), demonstrating enhanced charge-trapping capability and surface potential, resulting in much higher output from the TENG compared to its counterpart. The integration of CuICuII-1 with ethylcellulose enhanced the electrical efficiency of the composite, resulting in elevated current and voltage outputs. Several TENG units were subsequently interconnected to capture biomechanical energy and power LEDs, thereby facilitating photocatalytic processes such as C(sp)–H/Si–H coupling (Fig. 13c). In addition, quadruple M-TENG devices were engineered as autonomous smart flooring systems capable of transforming human movement into useful electrical energy. When combined with signal-processing and control units, these systems can immediately energize household equipment such as thermohygrometers, calculators, and LEDs without the need for additional energy storage. The stored mechanical energy enables continuous light production, thereby supporting applications such as selective photochemical processes and demonstrating its potential for smart homes and self-sustaining functional systems (Fig. 13d). Their study emphasizes that ML-assisted design of multifunctional MOFs facilitates effective energy harvesting, storage, and usage on a unified platform, hence advancing scalable self-powered photocatalytic systems and sustainable electronic applications.

6. Challenges and limitations

Despite notable advancements, various challenges impede the complete realization of AI and ML in materials and device research.

6.1. Data scarcity, bias, and reproducibility

High-quality, large datasets remain a significant limitation. Numerous emerging materials and device structures, especially perovskite photovoltaics, solid-state batteries, and multifunctional optoelectronic devices, lack sufficient experimental and computational data. This shortage diminishes the reliability of model estimates and may lead to overfitting or inadequate generalization [153]. Data bias, arising from the overrepresentation of certain materials classes, experimental protocols, or favored synthesis methods, can distort predictions and limit applicability to wider systems. Reproducibility issues intensify these difficulties; variations in experimental setups, evaluation approaches, and computational coefficients can result in discrepancies between model predictions and laboratory results [154]. Resolving these issues requires standardized datasets, open-access repositories, robust benchmarking protocols, and uncertainty quantification and error-propagation techniques to enhance confidence in AI-driven predictions.

6.2. Generalization across materials and devices

AI models frequently struggle to generalize beyond their training data. Models developed for lithium-ion battery electrodes may exhibit suboptimal performance when applied to sodium-ion or solid-state systems [155]. Similarly, models trained on silicon-based photovoltaics may not accurately predict the behavior of perovskite or organic alternatives. Broad generalization can be achieved through techniques such as transfer learning, domain adaptation, and hybrid physics-informed models that combine first-principles understanding with data-driven methods [156]. The absence of these methods limits the application of AI across various materials and devices, thereby constraining its potential to enhance discovery and performance in emerging technologies.

6.3. Interpretability versus accuracy trade-offs

Complex deep learning algorithms, despite their power, frequently operate as “black boxes,” offering minimal insight into the fundamental physics or chemistry of material structures. This opacity diminishes their impact in informing experimental development and mechanistic comprehension [157]. In contrast, simpler models such as linear regression or decision trees offer interpretability but may not adequately capture the nonlinear interactions essential to device performance [158]. The challenge of balancing interpretability and predictive accuracy remains ongoing. Recent methodologies, such as explainable AI methods, surrogate modeling, and feature significance analysis, offer viable solutions that deliver actionable insights while maintaining performance. However, broader adoption and standardization remain necessary [159].

6.4. Bridging computational predictions and experiments

Despite models achieving high predictive accuracy, converting these predictions into reproducible experimental results remains a considerable challenge. Numerous predicted materials pose challenges during synthesis or exhibit stability concerns in practical environments [160]. The transition from computational predictions to device-level production presents challenges, including processing constraints, defect management, and adaptability to environmental factors [161]. Addressing this gap necessitates iterative and unified workflows that closely link computational modeling and AI-driven predictions with experimental approaches for rapid validation and feedback mechanisms to enhance both models and synthesis protocols [162].

6.5. Summary and practical recommendations

Overall, the reviewed studies show that the primary challenges in AI and ML for materials and device research are data limitations, generalization constraints, interpretability trade-offs, and translation gaps across experiments. Confronting these challenges requires specialized strategies, such as generating standardized, high-quality datasets (e.g., Materials Project, OMEAD), implementing transfer learning and physics-informed models to enhance generalization, and incorporating explainable AI techniques to elucidate critical structural and chemical descriptors. Iterative methods that connect computational predictions to swift experimental validation have been shown to enhance materials discovery, as evidenced by research on sodium-ion cathodes [77], hybrid supercapacitors [86], and organic electrodes [93]. Future research should emphasize multimodal datasets that include structural, electrochemical, and environmental properties, while implementing cohesive pipelines that link data-driven modeling with experimental design. These methodologies will improve predictive accuracy, aid mechanistic understanding, and enable the conversion of AI-generated findings into functional, high-performance materials and technologies. Scheme 4 outlines the main challenges and limitations of AI and ML in the research of materials and energy devices, accompanied with domain-specific techniques extracted from the analyzed studies. Data scarcity and bias, common in emerging materials like perovskites and solid-state battery electrodes, diminish predictive reliability and may lead to overfitting. Restricted generalization hinders models trained on specific systems from achieving optimal performance with novel materials, as demonstrated in experiments comparing Li-ion and Na-ion batteries. Compromises between interpretability and predictive accuracy can confound mechanical understanding, especially in deep learning applications such as graph neural networks for voltage forecasting. Connecting computational predictions to experimental outcomes remains a significant problem, necessitating iterative workflows that integrate data-driven models with swift experimental validation, as evidenced in research on hybrid supercapacitors and organic electrodes. This schematic provides a visual roadmap of these challenges, their consequences, and actionable strategies, enhancing clarity for readers and highlighting practical approaches to accelerate AI-driven materials discovery.

7. Future outlook

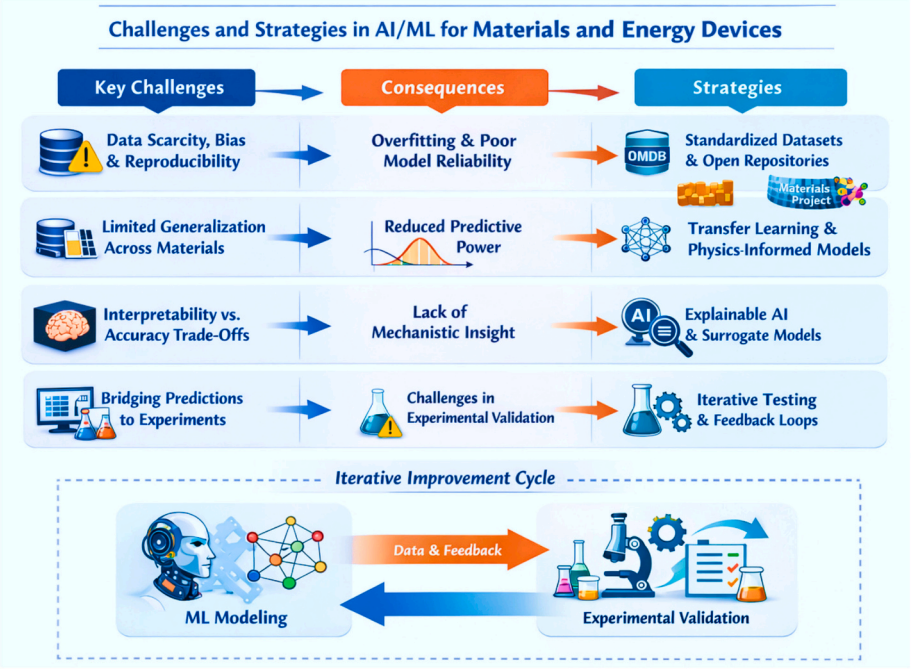
The integration of AI, ML, and novel experimental and computational methodologies presents significant advancements in materials and device research.

7.1. Autonomous laboratories and closed-loop experimentation

Autonomous laboratories that incorporate robotics, high-throughput formulation, and AI-based decision-making can accelerate discovery cycles. In closed-loop systems, AI models can iteratively design, execute, and analyze experiments, refining predictions in real time. These systems minimize human intervention, enhance reproducibility, and facilitate the swift optimization of multifunctional materials and devices.

7.2. Quantum computing–enhanced AI for materials discovery

Quantum computing offers the potential to simulate intricate electronic, structural, and thermodynamic processes that are computationally infeasible using classical approaches. AI integration with quantum-enhanced simulations enables exploration of extensive chemical and structural spaces, supports accurate predictions of device architectures,



Scheme 4. Schematic overview of key challenges, consequences, and strategies in AI/ML for materials and energy devices.

and facilitates the discovery of innovative materials for energy storage, photovoltaics, and multifunctional optoelectronics.

7.3. Sustainable and green AI approaches

Large-scale AI and ML applications impose significant computational demands, resulting in increased energy consumption and environmental effects. Future research should emphasize sustainable strategies, such as energy-efficient methods, cost-effective surrogate models, and cloud-based, renewable-energy-powered high-performance computing. Data-efficient methods that reduce reliance on large experimental or simulation datasets can decrease computational demands while preserving predictive accuracy.

7.4. Industrial translation and commercialization

The translation of AI-discovered materials and device concepts into industrial-scale applications presents a significant challenge. Considerations include manufacturability, cost, scalability, and compliance with regulatory standards. AI can enhance industrial translation by predicting scalable synthesis pathways, enhancing process parameters, and predicting long-term performance under operational conditions. The effective integration of AI into industrial R&D processes could greatly expedite the commercialization and adoption of advanced energy technologies.

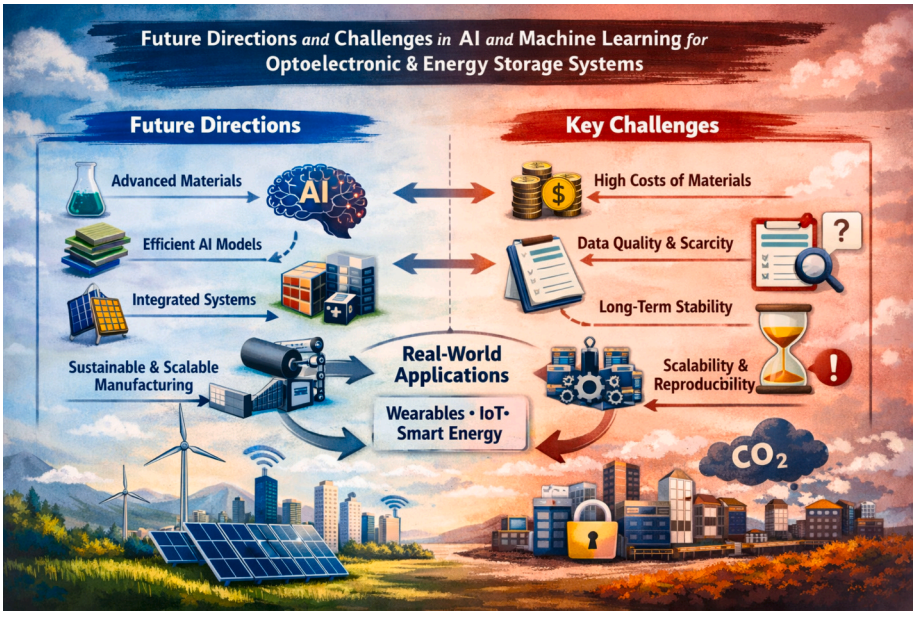
7.5. Industrial translation and commercialization

Although AI and ML have significantly accelerated materials discovery and device optimization, their effective use requires a thorough techno-economic assessment. Significant challenges include elevated costs, complex synthesis of advanced materials such as MXenes and MOFs, and concerns about scalability, repeatability, and long-term stability. Ensuring compatibility with scalable processes, such as solution-based and roll-to-roll approaches, is important for commercialization. Moreover, whereas ML reduces experimental effort, it incurs computational and data-related costs that must be weighed against efficiency gains. From an application standpoint, the balance between cost and performance is essential, as economically feasible systems often prioritize scalable and moderately optimized architectures. Nonetheless, AI-driven optoelectronic and energy storage technologies hold significant promise for wearable electronics, IoT systems, and smart energy devices, contingent on the development of cost-effective materials, efficient models, and industry integration. In addition, a Scheme 5 for future directions is provided, illustrating the key challenges and emerging opportunities of AI and ML in optoelectronic and energy storage systems, including material design, charge-transport optimization, interfacial engineering, scalability, and device stability for next-generation applications.

8. Conclusions

This review has presented a comprehensive and coherent perspective on the transformative impact of artificial intelligence (AI) and machine learning (ML) in optoelectronics and energy storage, bridging the gap from fundamental materials design to device-level applications. By outlining the foundations of ML, including core algorithms, data acquisition, feature engineering, and interpretable modeling, it becomes clear that the reliability of AI-driven predictions is strongly dependent on high-quality data and physically meaningful descriptors. The integration of domain knowledge into ML structure has emerged as a key factor in improving model robustness, transferability, and scientific interpretability. Significant progress has been achieved in optoelectronic devices, where ML has enabled rapid optimization of material compositions and device architectures in photovoltaics, light-emitting devices, and photodetectors. In parallel, energy storage technologies, including batteries, supercapacitors, and hybrid systems, have benefited from data-driven discovery of advanced electrode and electrolyte materials, as well as predictive modeling of electrochemical performance and degradation mechanisms. The growing convergence of these domains is evident in cross-cutting applications such as coupled optoelectronic–energy storage systems, inverse design strategies, and AI-enhanced multiphysics simulations. Emerging hybrid architectures, including TENG–supercapacitor systems based on MXene–MOF–chalcogenide materials, further underscore the potential of AI in designing multifunctional, next-generation energy platforms.

Despite these advances, key challenges persist. Data scarcity, bias, and reproducibility issues limit the generalizability of ML models, particularly for emerging materials systems. The trade-off between interpretability and predictive accuracy remains a central concern, while the gap between computational predictions and experimental realization continues to hinder practical implementation. Addressing



Scheme 5. Schematic illustration of the key challenges and future directions of AI and ML in optoelectronic and energy storage systems.

these challenges requires standardized datasets, explainable AI approaches, and hybrid physics-informed models, along with iterative structures that integrate ML predictions with experimental validation. Looking ahead, the integration of AI with autonomous laboratories, quantum computing, and sustainable data practices is expected to redefine materials research and accelerate innovation. This review provides a unified and forward-looking structure that connects materials design, data-driven modeling, and device engineering, offering valuable insights for researchers across disciplines. By systematically integrating advances in optoelectronics and energy storage, it highlights emerging opportunities, identifies critical bottlenecks, and proposes actionable strategies for future development. Ultimately, this work serves as a guiding reference for advancing intelligent, high-performance, and sustainable technologies and is expected to help shape the next generation of AI-driven materials and energy systems.

Authors contribution

The manuscript was written with contributions from all authors. All authors have approved the final version of the manuscript.

Declaration of generative AI and AI-assisted technologies in the manuscript preparation process

During the preparation of this work, we used *ChatGPT* to assist with language refinement, improving clarity, structuring sentences, and enhancing the overall readability of the manuscript. After using this tool, we carefully reviewed, revised, and validated the content to ensure accuracy and originality, and we take full responsibility for the final published manuscript.

CRediT authorship contribution statement

Yunsheng Zhang: Writing – original draft, Visualization, Data curation, Conceptualization. **Muhammad Sadiq:** Writing – review & editing, Supervision, Funding acquisition, Formal analysis, Data curation. **Muhammad Moazam Fraz:** Software, Resources. **Eman Ali Aldhahri:** Methodology, Investigation. **Abdulwahab Ali Almazroi:** Methodology, Investigation. **Mariam Iqbal:** Methodology, Investigation. **Asif Hayat:** Software, Resources. **Yu Geng:** Methodology, Investigation. **Ahmed S. Algamdi:** Project administration, Methodology. **Amber Noreen:** Software, Resources. **Aiman Fatima:** Methodology, Investigation. **Junwei Liang:** Writing – review & editing, Methodology, Investigation, Funding acquisition. **Hamid Ali:** Writing – review & editing, Visualization, Supervision, Methodology, Investigation, Funding acquisition.

Declaration of competing interest

The authors declare that no known financial or personal conflicts of interest could have influenced the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.susmat.2026.e01949.

Data availability

The data will be available on request.

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