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REVIEW ARTICLE

Toward intelligent design of solid-state hydrogen storage: trends, challenges, and machine learning insights

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Abstract Solid-state hydrogen storage is widely recognized as a promising pathway for safe, high-density, and reversible hydrogen utilization, yet its advancement remains hampered by complex thermodynamic, kinetic, and structural constraints. This review highlights the emerging role of big data and machine learning in reshaping the research landscape. Through analyses enabled by the Digital Hydrogen-S platform, recent material development trends and persistent bottlenecks are systematically identified, revealing widespread misalignments with the US Department of Energy targets in storage capacity, operating temperature, and pressure. Data-driven approaches are shown to accelerate property prediction, high-throughput screening, and inverse design, while the integration with high-throughput computation and experimental validation is forming an intelligent closed-loop paradigm. Meanwhile, neural network potentials offer near-first-principles accuracy for probing hydrogen adsorption, dissociation, and diffusion, though challenges in long-range interactions and transferability remain. Looking ahead, establishing open-access multimodal databases (combining numbers, text, spectra, and images), developing multimodal large language models, implementing inverse design strategies, and constructing generalized neural network potentials capable of describing complete absorption-desorption cycles represent critical steps toward intelligent and practical material discovery. This review provides a structured framework to guide future research and accelerate the deployment of solid-state hydrogen storage technologies.

Keywords solid-state hydrogen storage, data-driven materials design, machine learning neural network potentials

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1 Introduction

Hydrogen, with its much higher gravimetric energy density compared to conventional fossil fuels and its zero-carbon emission property, is broadly recognized as a crucial energy vector for realizing the clean energy transition and carbon neutrality goals [1−3]. Nevertheless, the large-scale application of hydrogen is still constrained by storage and transportation technologies [4]. Currently, hydrogen storage methods mainly include high-pressure gaseous storage, cryogenic liquid storage, and solid-state storage [5]. Specifically, high-pressure gas storage suffers from low energy density and safety concerns [6], while cryogenic liquid storage provides higher energy density but demands extremely low temperatures, resulting in high energy consumption and elevated costs [7]. In contrast, solid-state hydrogen storage is viewed as a promising pathway for future hydrogen utilization, owing to its higher volumetric density, enhanced safety, and relatively moderate operating temperature and pressure conditions [8,9]. The realization of large-scale applications, however, hinges on the sustained development of high-performance solid-state hydrogen storage materials, thereby positioning materials research as a pivotal driver of the hydrogen economy [10].

Solid-state hydrogen storage research has traditionally employed multiple approaches, such as experimental investigations [11], thermodynamic modeling [12], and first-principles calculations [13]. As the most straightforward method, experimental research yields the actual performance parameters of materials and provides a robust basis for material screening and mechanistic investigation [14]. Nevertheless, the process is typically resource-intensive and time-consuming, and it is difficult to systematically encompass all potential material combinations in complex systems [15]. Zhu et al. [16] developed a temperature-variable cycling (TVC) screening device to overcome the limitations of accuracy and efficiency in conventional volumetric equipment. This system can effectively carry out TVC pressure-composition-temperature (PCT), TVC kinetic, and temperature-programmed desorption/adsorption measurements; nonetheless, completing one TVC PCT test (three PCT curves) still takes about 1.5 days [16]. To overcome the time and scale limitations of conventional experimental screening, thermodynamic modeling (such as calculation of phase diagrams) has been extensively introduced to predict phase equilibria and thermodynamic properties of hydrogen storage [17]. However, the predictive accuracy of such methods is heavily dependent on thermodynamic databases, model assumptions, and fitted parameters, and decreases markedly when applied to multicomponent or extrapolated systems [18]. With the advancement of computational materials science, first-principles calculations have become a crucial tool for solid-state hydrogen storage research, offering insights into the underlying hydrogen storage mechanisms from the perspective of electronic structure [19]. Nonetheless, first-principles calculations involve substantial computational cost and are constrained by time-scale and system-size limitations; while they can elucidate dynamic mechanisms, they are typically restricted to short temporal spans and relatively small systems [20,21]. In summary, while traditional approaches have provided a foundation for solid-state hydrogen storage studies, their inherent limitations in efficiency, scope, and predictive power render them inadequate to meet the current urgent demand for rapid material design and performance optimization.

With the improvement of computational power and the continuous accumulation of data resources, data-driven approaches are increasingly being introduced into the study of solid-state hydrogen storage [22]. Big data analytics enables researchers to identify patterns from diverse experimental and computational data sets, whereas machine learning (ML) offers novel pathways to map the relationships between material structures and their properties [23]. In recent years, related studies have demonstrated that ML cannot only accelerate performance prediction but also gradually extend to applications in material design. For instance, Verma et al. [24] developed the HEART ML framework to predict hydrogen storage capacity and hydride formation enthalpy in multicomponent alloys. After evaluating about 6.4 million binary, ternary, and quaternary alloy combinations from 38 elements, they screened out 6480 potential candidates that satisfy the US Department of Energy (DOE) criteria (H_2 wt % > 2.5 and $\Delta H < 60$ kJ·mol^{-1} H_2 under room conditions). Similarly, Bhattacharjee et al. [25] employed a hybrid ML strategy combining autoencoders and deep neural networks (DNNs), which significantly improved the prediction accuracy of hydrogen storage capacity in metal hydrides under limited data conditions. Furthermore, Dangwal et al. [26] combined Gaussian process regression (GPR) with experimental and first-principles based on density functional theory (DFT) data to explore high-entropy alloys (HEAs), achieving reliable prediction of hydride formation enthalpies close to room temperature. Meanwhile, researchers have integrated ML with high-throughput screening to identify metal-organic frameworks (MOFs) structures that possess both high hydrogen storage capacity and synthetic feasibility, and validated these predictions through the successful synthesis of a V-based MOF [27]. Collectively, these achievements indicate that data-driven methods are likely to break through the bottlenecks of traditional research methods and inject new momentum into the development of solid-state hydrogen storage materials.

However, research on solid-state hydrogen storage remains hindered by limited data, inconsistent experimental protocols, and challenges in model transferability and interpretability. On this basis, this review aims to systematically summarize the latest progress in solid-state hydrogen storage and provide new perspectives. More specifically, our discussion begins with the Digital Hydrogen-S platform, through which we analyze the development and challenges of solid-state hydrogen storage materials from the perspective of data followed by an overview of both the advancements and shortcomings of applying ML to solid-state hydrogen storage research and design; then, we will examine how neural network potentials (NNPs) have been applied to reveal the mechanisms of hydrogen uptake and release, along with their inherent limitations; and ultimately, we offer perspectives on promising directions for future research. With this review, our goal is to furnish the community with a structured reference that may foster the efficient design of solid-state hydrogen storage materials and accelerate the real-world deployment of hydrogen technologies.

2 Developments and challenges in solid-state hydrogen storage: a data-centric perspective

2.1 Data sources and the Digital Hydrogen-S platform

Experimental data serve as the cornerstone of data-driven research. However, hydrogen storage measurements obtained under different instruments, testing procedures, and standard conditions often exhibit certain variability, introducing data noise that may influence the reliability of subsequent analysis and modeling [28]. While moderate noise can improve a model's generalization by mitigating overfitting, excessive noise distorts intrinsic correlations and may lead to model failure [29]. These deficiencies not only limit the effectiveness of artificial intelligence (AI) and ML approaches but also hinder the systematic exploitation of experimental and computational results. Accordingly, the establishment of standardized, high-quality, multimodal, and well-curated databases is essential to ensure data consistency, traceability, and reusability, thereby providing a solid foundation for accelerating research and innovation in solid-state hydrogen storage. In this context, a systematic overview of existing hydrogen storage databases is both timely and imperative.

Currently, several significant hydrogen storage material databases have been developed globally, offering valuable resources for research, yet their overall development is still at an early stage. The HydPARK database [30], which is widely used internationally, primarily contains a narrow set of performance parameters such as chemical composition, hydrogen capacity, enthalpy of formation, operating temperature, and plateau pressure under ambient conditions. Nevertheless, the database suffers from limited coverage and has not shown any public updates or data expansions since its last recorded release in 2002 (verified as of September 2025), resulting in incomplete and outdated data. The Materials Project platform [31] provides thermodynamic data for certain metal hydrides, which are mainly obtained from high-throughput computations, while experimental conditions, synthesis details, and characterization data are missing. The database established by the Dalian Institute of Chemical Physics (CAS) primarily records optimal hydrogen storage capacities and plateau pressures at designated temperatures, and incorporates a ‘preparation method’ field; however, this entry remains superficial, limited to method names, and lacks experimental data, resulting in considerable omissions [32]. In parallel, Japan’s National Institute for Materials Science (NIMS) has released partial open data sets related to alloy hydrogen storage properties, yet these data sets are largely confined to numerical thermodynamic values and cycling stability, with relatively narrow scope [33]. Furthermore, the team led by Lixian Sun [34] at Guilin University of Electronic Technology developed a new hydrogen storage database leveraging AI-powered tools for literature data collection and management, incorporating numerical physicochemical descriptors including composition, structure, atomic number, and atomic radius [34]. However, the database lacks multimodal information, particularly characterization data (e.g., X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and transmission electron microscopy (TEM) images) and synthesis-related details, which limits its ability to provide a complete and systematic collection. Overall, while these databases offer valuable references for investigating and comparing hydrogen storage materials, notable shortcomings remain in their breadth, comprehensiveness, and depth, limiting their ability to satisfy present research demands.

Beyond publicly accessible databases, numerous research groups have constructed their own data sets in the context of AI-driven hydrogen storage studies, primarily for model training and property prediction. For instance, Lu et al. [35] built a structure-property relationship model of V-Ti-Cr-Fe alloys based on 81 samples and 19 features to predict maximum hydrogen absorption capacity. Owing to the small data set and the exclusive use of numerical descriptors, the model exhibited restricted generalizability. Dong et al. [36] collected 826 samples with 47 descriptors to predict the hydrogen storage performance of Mg-based alloys. Despite the inclusion of certain process-related attributes, the data set was still confined mainly to numerical information. Zhou et al. [37] created a data set of 234 C14 Laves-type HEAs covering alloy composition along with thermodynamic and kinetic properties, yet the absence of spectroscopic and microstructural data remained a limitation. Kim et al. [38] collected 506 raw PCT data points at 303 K for 33 AB_2-type alloys and employed ML models to predict absorption/desorption curves across different temperatures. Still, the features used were restricted to composition, temperature, and pressure, and the data set size was insufficient to capture synthesis and characterization details. In summary, while these group-specific databases have facilitated progress in targeted applications, they still commonly face constraints of small data set sizes and unimodal information, hindering both model generalization and deeper mechanistic insights.

Despite these efforts, both publicly available and small-group databases often face limitations in coverage, completeness, and data modality, highlighting the urgent need for more comprehensive platforms. To meet these challenges, the Hydrogen Science and Engineering team at North China Electric Power University developed the Digital Hydrogen-S data platform [39], as shown in Fig. 1(a). In contrast to earlier databases focused largely on numerical attributes, as shown Table 1, this platform highlights the integration of multimodal and structured data as a core design principle. It consolidates data from more than 1000 peer-reviewed publications, comprising over 3000 unique material entries and exceeding 254000 structured records. These span ten major classes of hydrogen storage materials, such as Mg-based hydrides, AB_5 alloys, HEAs, borohydrides (BH_4), and MOFs. Notably, beyond chemical compositions and thermodynamic data, the platform systematically incorporates experimental PCT curves, kinetic curves, and synthesis parameters, thereby establishing a multimodal data architecture. Moreover, the platform employs a DOI-centered hierarchical information architecture (see Fig. 1(b)). The database consists of three layers: the first records basic bibliographic information; the second contains detailed material data and associated curve files;

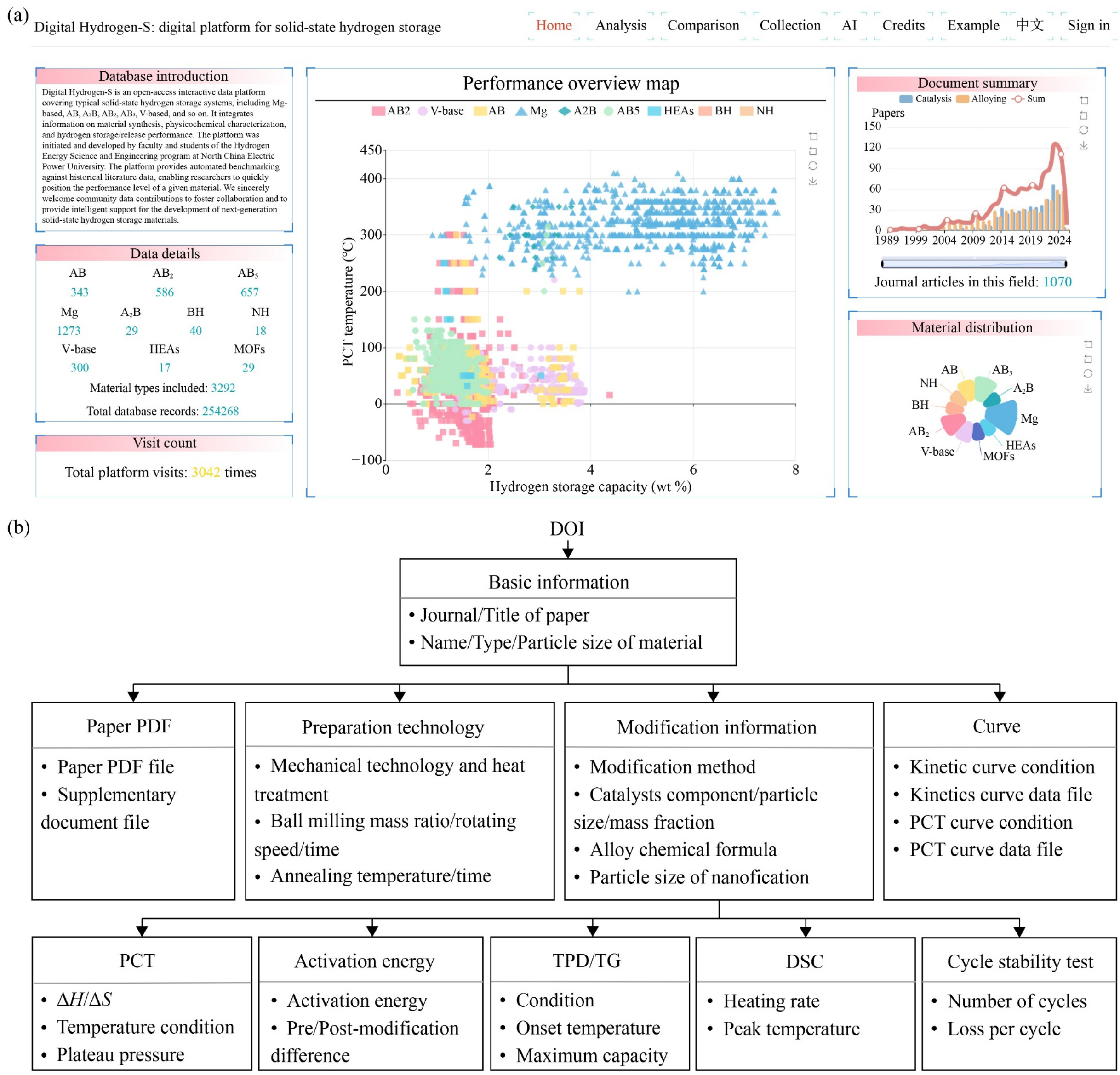

Fig. 1 Digital Hydrogen-S data platform. (a) Homepage; (b) Database structure; (c) Temporal distribution of publications for Mg-based, V-based, AB, A_2B, and AB_2 hydrogen storage materials; (d) Temporal distribution of publications for AB_5, BH_4, NH_4, HEAs, and MOFs hydrogen storage materials.

Table 1 Comparison of major hydrogen storage databases

Database	Release year	Data modality	Data type	Ref.
HydPARK	2001	Single-modal	Experimental data (thermodynamic/performance values)	[30]
Materials project	2010	Single-modal	Computed DFT data (structures, energies, and electronic properties values)	[33]
NIMS materials database	2010	Single-modal	Experimental property data sets/engineering property sheets	[32]
DICP hydrogen storage database	2011	Single-modal	Experimental data (performance values)	[31]
Digital Hydrogen-S	2025	Multi-modal	Experimental data (thermodynamic/kinetic data, PCT curves, kinetic curves, and synthesis metadata)	[39]

and the third systematically documents hydrogen absorption/desorption performance parameters. This layered design ensures the systematic and complete documentation of each entry during data recording. Owing to its multimodal data sets and strict structured framework, the platform offers enriched and reliable input features for ML and data-driven approaches. As data continue to accumulate and be updated, Digital Hydrogen-S has the potential to become a crucial tool in advancing solid-state hydrogen storage studies.

2.2 Trends in material development based on data statistics

Data statistics provide a fundamental means to examine research progress, as they offer objective insights into temporal evolution, research priorities, and emerging directions. With the continuous accumulation of structured data, it becomes feasible to quantitatively identify trends in hydrogen storage materials and to interpret their underlying drivers. Drawing on bibliometric evidence and database-derived statistics, this section outlines the research trajectory of hydrogen storage materials over the past decade and a half.

Building on this perspective, bibliometric analysis of publications retrieved from the Web of Science Core Collection provides a clear view of how research in hydrogen storage materials has evolved over time. Using ‘hydrogen storage materials’ as the topic keyword, articles published between 2010 and 2024 were collected, revealing a continuous growth in the number of publications from 1490 in 2010 to 11031 in 2024. A particularly rapid increase occurred after 2016, with marked surges in 2022 (8910 articles) and 2023 (10510 articles). Such accelerated growth clearly reflects the intensified global research interest in hydrogen energy, particularly in solid-state storage, driven by rising demand for sustainable energy, breakthroughs in material synthesis, and the increasing availability of computational tools. Previous studies have similarly highlighted this trend, attributing it to both technological advances and policy-driven incentives for hydrogen energy [40,41].

To provide a more focused perspective, publication trends for solid-state hydrogen storage materials were further examined using records collected from the digital hydrogen-S data platform. The number of peer-reviewed publications recorded in this platform increased from 16 in 2010 to 107 in 2024, showing a broadly similar upward trajectory to that observed in the Web of Science data set, though with a considerably smaller scale. A notable discrepancy is observed in the years 2023–2024, where the platform data indicate a decline from 123 to 107 entries, in contrast to the continued growth seen in the Web of Science results. This difference can be attributed to the broader coverage of the Web of Science database as well as the fact that the Digital Hydrogen-S platform is still under development and has not yet fully incorporated the most recent publications. Despite these deviations, the overall consistency between the two data sets lends credibility to the bibliometric statistics provided by the platform, thereby establishing a robust foundation for subsequent analyses of material-specific research trends.

Extending from this overall perspective, Figs. 2(a) and 2(b) provide a closer examination of the temporal distributions of different hydrogen-storage material classes curated in the Digital Hydrogen-S platform, thereby linking publication dynamics at the field level to material-specific research trajectories. For Mg-based materials, data points become densely distributed after 2010, and the median publication year is close to 2020, indicating sustained research intensity over the past decade. Vanadium solid solutions (V-based) exhibit a wide temporal span with earliest reports traceable to the 1990s, yet the majority of publications cluster after 2010, and the median likewise approaches 2020, suggesting renewed attention in recent years. AB and A_2B alloys are predominantly reported in the post-2010 period, with A_2B alloys showing relatively lower research intensity. AB_2 alloys, like vanadium solid solutions, have long research histories extending before 1990, but most documented activity in the platform is concentrated in the last decade.

Turning to the material classes shown in Fig. 1(d), AB_5 alloys display the broadest temporal coverage, with active research since the early 2000s and sustained prominence through 2010–2025, reflecting their maturity and continued relevance. BH_4 is mainly recorded after 2010 with a peak around 2015, indicating episodic but notable interest. Nitrogen-hydrogen compounds (NH_4) have too few data points to reliably reflect their actual research status. A complementary search in the Web of Science database shows that their application in the solid-state hydrogen storage field remains limited, making it difficult to determine a clear developmental trajectory. HEAs emerged primarily after 2015, with a median near 2020, marking a rapidly growing direction. Although the number of HEA data points in the figure is limited, the overall pattern does align with the broader research trend. Previous studies have noted that following the first report on hydrogen storage properties of HEAs in 2010, only a few papers were published in the subsequent five years, while interest in this field has notably increased since 2016 [42]. MOFs appear in the platform from around 2000, but with relatively few and dispersed entries; this likely reflects incomplete MOFs coverage in the current

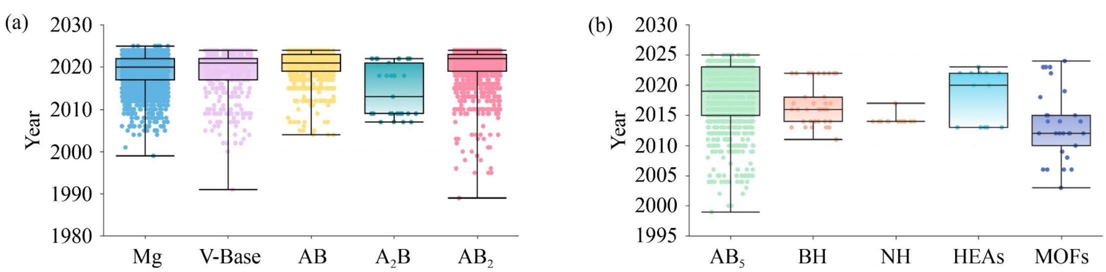

Fig. 2 (a) Temporal distribution of publications for Mg-based, V-based, AB, A_2B, and AB_2 hydrogen storage materials; (b) Temporal distribution of publications for AB_5, BH_4, NH_4, HEAs, and MOFs hydrogen storage materials.

database rather than an actual paucity of MOFs research in the literature.

Collectively, while several classical alloy systems (e.g., Mg-based, vanadium solid solutions, AB_2) have long research histories, their recent research momentum is concentrated within the past decade. At the same time, emerging material classes such as HEAs and NH_4 have only begun to attract significant attention in recent years, whereas BH_4 and MOFs show more episodic or dispersed patterns of activity. Taken together, these patterns indicate that the field of solid-state hydrogen storage is characterized by both the sustained evolution of conventional alloys and the gradual emergence of novel material systems, reflecting a diversified trajectory of development.

2.3 Challenges identified through data analytics

Although continuous progress has been achieved, solid-state hydrogen storage materials still face considerable challenges in meeting practical requirements. In practical applications, the key performance parameters of concern such as gravimetric hydrogen storage capacity, operating temperature, delivery pressure, and cycling stability. The DOE has introduced the Technical Targets for Onboard Hydrogen Storage for Light-Duty Vehicles [43], which serve as key references for evaluating the performance of hydrogen storage materials. Among these performance indicators, the DOE has set targets including gravimetric hydrogen storage capacities of 5.5 wt % by 2025 and 6.5 wt % as a long-term goal, as well as an acceptable operating ambient temperature range of –40 to 60 °C, minimum/maximum delivery temperatures of –40 to 85 °C, and a delivery pressure window of 5–12 bar. In particular, the delivery temperature constraint explicitly defines the allowable range for hydrogen at the system outlet, meaning that the intrinsic hydrogen absorption and desorption characteristics of the material must align with this window to enable effective system operation without the need for additional complex thermal management. Similarly, the delivery pressure constraint sets the acceptable boundaries for system integration, highlighting the necessity for candidate materials to exhibit equilibrium pressures compatible with practical onboard conditions.

Lu et al. [44] established a large-scale hydride database comprising more than 1000 alloys and 6000 valid records, with all data uploaded in the Digital Hydrogen-S platform. By applying unsupervised K-means clustering to three key parameters (hydrogen storage capacity, plateau pressure, and operating temperature), their analysis yielded three distinct clusters, as shown in Fig. 3(a). Figures 3(b–d) further provide alternative two-dimensional projections of these distributions. The clustering results divide the materials into three categories: Cluster 0 mainly consists of V-Ti-Cr-based alloys; Cluster 1 is dominated by Mg-rare earth (RE)-Ni systems; while Cluster 2 corresponds primarily to Ti-Fe- and Ti-Mn-based alloys. The following discussion summarizes the performance characteristics of these alloy classes based on the combined insights from Figs. 3(a–d).

V-Ti-Cr alloys generally exhibit moderate hydrogen storage capacities, mostly within 1–4 wt %. Their operating temperatures are mainly distributed between –23 and 127 °C, which is close to the DOE delivery temperature window of –40 to 85 °C. In terms of plateau pressure, most data points are located below 50 bar, which still exceeds the DOE requirement of 5–12 bar for onboard systems. Overall, although these alloys possess relatively suitable thermal characteristics, their gravimetric hydrogen storage capacities are far below the DOE targets of 5.5 wt % (2025) and 6.5 wt % (ultimate). The main challenge therefore lies in their insufficient storage density.

Mg-RE-Ni alloys show significantly higher gravimetric hydrogen storage capacities, with several data points exceeding 6–7 wt %, thereby reaching or even surpassing the DOE targets. Their plateau pressures are generally below 2 MPa, which falls within or near the DOE delivery pressure range. However, their operating temperatures are concentrated above 500 K, which is far beyond the DOE delivery window of –40 to 85 °C. As a result, the major limitation of these alloys lies in their excessively high dehydrogenation temperatures, which severely restricts their practical use in onboard storage systems.

Ti-Fe and Ti-Mn alloys are characterized by relatively low hydrogen storage capacities, typically below 2 wt %. Their operating temperatures fall within the moderate range of 300–350 K, which is compatible with the DOE delivery window. However, their plateau pressures are often above 10 MPa, which is far higher than the DOE target of 5–12 bar. Consequently, despite acceptable operating temperatures, these alloys are unsuitable for onboard hydrogen storage due to the dual challenges of low hydrogen capacity and excessively high equilibrium pressures.

In summary, at present, almost no alloy materials can meet the DOE technical targets. V-Ti-Cr alloys suffer from insufficient gravimetric capacities, Mg-RE-Ni alloys are hindered by excessively high operating temperatures, and Ti-Fe/Ti-Mn alloys fail on both capacity and pressure. Beyond these individual discrepancies, a more systemic pattern emerges when examining the data distribution itself. The majority of hydride alloys are densely concentrated within limited regions of the capacity-temperature-pressure space, whereas vast portions of the performance domain remain sparsely populated or completely unexplored. Such uneven sampling distribution introduces a pronounced out-of-distribution (OOD) problem for data-driven modeling, where ML models trained on biased data sets struggle to generalize to unseen or underrepresented regions. Consequently, predictive reliability deteriorates when extrapolating toward materials or conditions beyond the

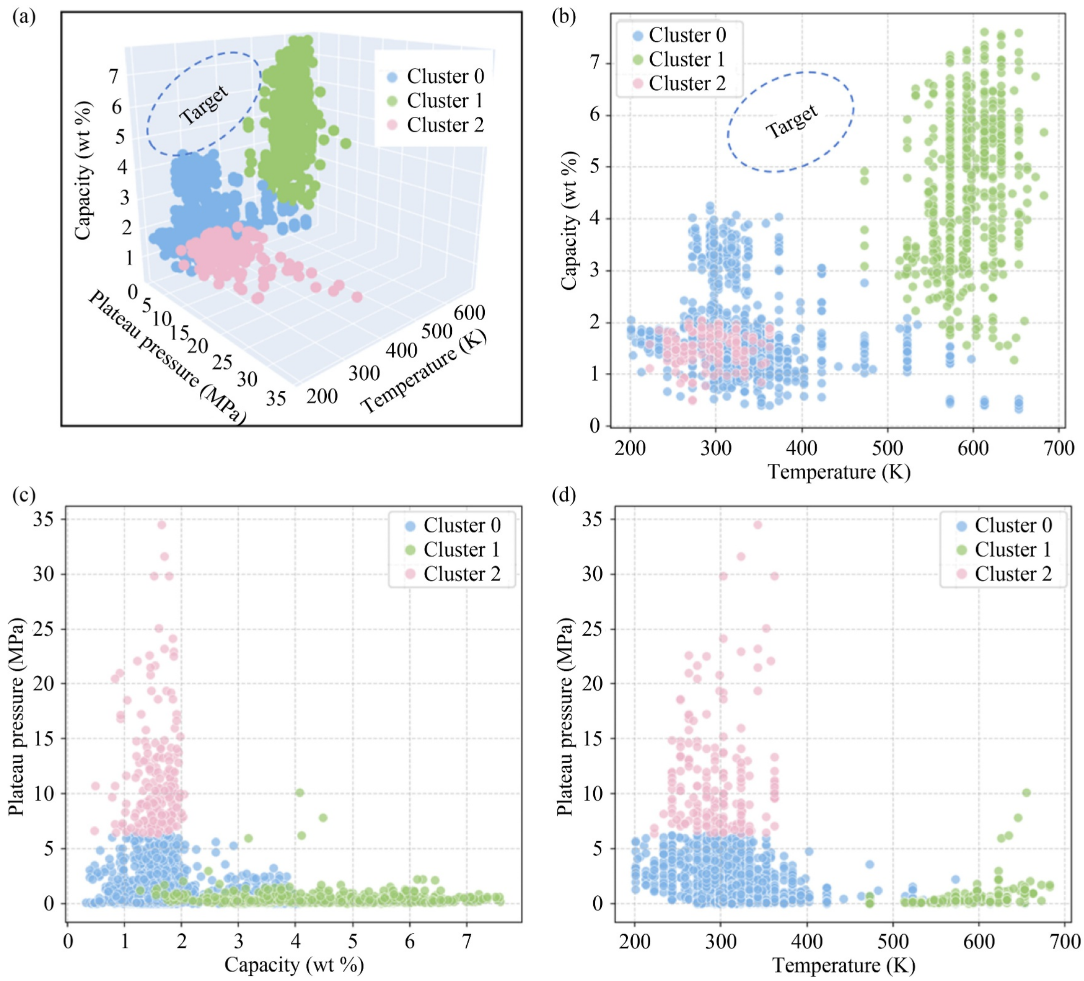

Fig. 3 Unsupervised clustering of data. (a) Three-dimensional (3D) K-Means clustering using the features 'Temperature', 'Plateau pressure', and 'Capacity'; (b) Side view of 3D clustering, features 'Capacity' and 'Temperature'; (c) Front view of 3D clustering, features 'Plateau pressure', and 'Capacity'; (d) Top view of 3D clustering, features 'Plateau pressure', and 'Temperature'. Reprinted with permission from Ref. [44], copyright 2025, Springer.

dominant data clusters. In other words, the predictive power of these models becomes increasingly uncertain as they move away from the data-rich zones. This systemic imbalance not only reflects intrinsic material limitations but also poses a fundamental challenge for building generalizable models. Therefore, to advance robust predictive modeling and enable reliable inverse design, it is necessary to expand the data set and systematically explore these sparse regions, which represents an essential step toward discovering solid-state hydrogen storage alloys that can satisfy integrated practical requirements.

3 ML for materials discovery in hydrogen storage

3.1 Data-driven material design framework

3.1.1 ML frameworks

As a vital component of AI, ML technology enables computer systems to learn through data analysis, thereby achieving predictive and decision-making capabilities for specific tasks [45]. Building upon these capabilities, ML methods demonstrate significant application potential in the efficient R&D of high-performance solid-state hydrogen storage materials. As illustrated in Fig. 4, the typical workflow of ML in materials science research can be divided into the following key stages: data set construction, feature extraction and engineering processing, model establishment and training, followed by model performance evaluation and practical application [46].

Database construction and standardized processing form the foundational work for ensuring model reliability. The widely used HydPARK database systematically compiles experimental measurement data and theoretical calculation results for AB-type, AB_2-type, AB_5-type, magnesium-based alloys, and complex hydride systems. However, due to uneven data distribution, variations in experimental conditions, and inconsistent data quality, this database faces numerous challenges when directly applied to ML modeling. To overcome these limitations,

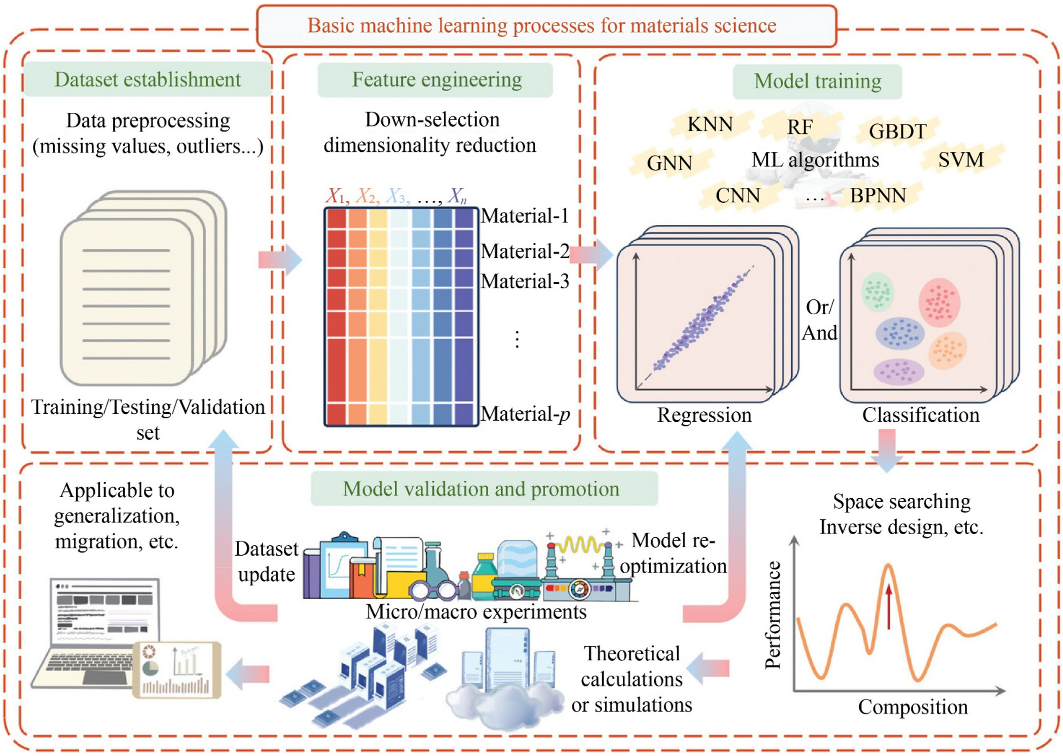

Fig. 4 ML workflow for hydrogen storage materials (GBDT: gradient boosting decision tree; BPNN: backpropagation neural network; CNN: convolutional neural network). Reprinted with permission from Ref. [49], copyright 2025, Wiley.

researchers developed optimized versions through systematic data cleaning, standardization, and quality control processes, significantly improving data set consistency and modeling applicability [47].

Feature engineering technology serves as the pivotal link connecting material microstructure with macroscopic properties, playing a central role throughout the framework. The descriptor system for hydrogen storage materials typically encompasses multiple levels: atomic radius, electronegativity, valence electron count, and other parameters at the fundamental atomic property level; state functions such as mixed entropy and mixed enthalpy at the thermodynamic level; and quantum chemical parameters like d-band center position and electron density distribution at the electronic structure level [48]. Furthermore, for specific hydrogen storage systems, physicochemical quantities directly related to hydrogen storage behavior must be incorporated, such as lattice volume change rate, chemical bond energy, and hydrogen atom adsorption energy. In HEA hydrogen storage systems, structural parameters like local lattice distortion and atomic packing fraction have been demonstrated to be closely correlated with hydrogen atom diffusion kinetics and thermodynamic binding stability. However, high-dimensional feature spaces often contain considerable redundancy, which can impair model generalization; therefore, applying feature selection and dimensionality reduction techniques is essential. Common approaches include recursive feature elimination (RFE), feature importance assessment based on random forests (RF), and principal component analysis (PCA). Zhou et al. [37] compressed an initial 145-dimensional feature space into 20 core descriptors using the RFE algorithm, thereby significantly enhancing computational efficiency and generalization performance while maintaining prediction accuracy.

The selection and optimization of model algorithms constitute the core technical component of framework implementation. Different ML algorithms exhibit distinct suitability characteristics when processing hydrogen storage material data. For example, classical algorithms such as support vector machines (SVM) and RF demonstrate robust performance on small sample data sets, whereas gradient boosting regression (GBR), GPR, and emerging graph neural network (GNN) techniques tend to achieve superior predictive accuracy and stability when handling large-scale complex data. Dangwal et al. [26] successfully predicted the hydrogenation reaction enthalpy of HEAs using the GPR algorithm, achieving high consistency between predictions and experimental data as well as first-principles calculations. In another representative case, Kim et al. [27] employed an ML screening strategy to identify promising MOF candidate materials, which led to the successful synthesis of a novel V-based MOF. This material achieved a hydrogen storage mass density of 9.0 wt % at 77 K and 150 bar, significantly outperforming conventional MOFs.

In summary, the data-driven ML framework establishes a comprehensive technical chain spanning from database construction to performance prediction by systematically integrating key technological elements such as data resources, feature engineering, and algorithm optimization. As illustrated in Fig. 4, this framework forms a self-consistent closed-loop system that provides robust technical support for the efficient discovery and performance optimization of novel hydrogen storage materials, thereby significantly accelerating the overall R&D process in this field.

3.1.2 Applications of ML models

The application of ML models in solid-state hydrogen storage materials research has evolved from the proof-of-concept stage to practical prediction, demonstrating significant advantages in quantitatively forecasting multiple key performance parameters. Such applications not only accelerate material performance evaluation processes but also provide reliable theoretical guidance for experimental design.

As the primary metric for evaluating hydrogen storage materials, accurate prediction of hydrogen storage capacity is crucial for material screening. Rahnama et al. [47] employed a GBDT model based on the HydPARK data set to predict hydrogen storage capacity for multiple material types, achieving a coefficient of determination (R^2) value of 0.83 with a mean absolute error (MAE) of only 0.003 wt % H_2. Feature importance analysis revealed that material category, temperature, and hydride formation enthalpy are the three most critical factors influencing hydrogen storage capacity, while specific chemical composition has a relatively minor impact. Salehi et al. [50] developed a Committee Machine Intelligence System (CMIS) by integrating six ML models (Multilayer Perceptron, SVM, RF, CatBoost, LightGBM, XGBoost) to predict the gravimetric hydrogen storage capacity of MOFs using 294 experimental data points. By applying the leverage method to eliminate 2.04% suspected outlier data, the CMIS model achieved exceptional performance with an overall R^2 of 0.982 and a root mean square error (RMSE) of 0.088. Sensitivity analysis confirmed that Brunauer-Emmett-Teller surface area, pore volume, pressure, and temperature contribute equally to the prediction, which is consistent with the physical mechanism of physisorption-dominated hydrogen storage. For thermodynamic parameters, Nations et al. [51] utilized an RF ensemble model to forecast the formation energy of arbitrary novel hydrides, achieving a mean squared error of 0.102 eV^2. This approach successfully identified potential high-performance combinations involving transition metals and lanthanide elements. Furthermore, the close agreement between model predictions and DFT calculations underscores the reliability of these ML methods.

For different types of hydrogen storage materials, researchers have developed specialized prediction models to enhance forecasting accuracy. In the case of titanium-based Laves-phase AB_2 hydrogen storage alloys, Gheytanzadeh et al. [52] employed a GPR model with exponential kernel functions to predict hydride formation enthalpy, achieving high accuracy with R^2 = 0.969 and a RMSE of only 2.501 $kJ\cdot mol^{-1}$ H_2 (Figs. 5(a–c)). Sensitivity analysis of this model revealed that Ti, Zr, Cr, and V exhibit the most significant influence on hydrogenation enthalpy (Figs. 5(d) and 5(e)). In the case of magnesium-based systems, Jiang et al. [53] applied a GBDT model that successfully predicted MgH_2 dehydrogenation temperature with R^2 = 0.95 and RMSE = 29.98 K. Through SHapley Additive exPlanations (SHAP) value analysis, the study identified the doping ratio and electronegativity as key factors influencing dehydrogenation temperature, thereby providing quantitative guidance for modifying magnesium-based materials. For MOFs, Shekhar and Chowdhury [54] developed a dual-model framework combining a feed-forward neural network (FNN) and an extremely randomized tree (ERT) to predict H_2 deliverable capacities. The FNN performed better for gravimetric capacity, while the ERT, improved by polynomial feature engineering, showed higher accuracy for volumetric capacity. The models were trained on 98695 MOFs from 19 databases and validated by grand canonical Monte Carlo (GCMC) simulations, which confirmed strong agreement between predictions and computational results. Similarly, Borja et al. [55] evaluated 13 ML algorithms to predict gravimetric/volumetric H_2 uptakes of 29608 real MOFs (77 K, 5–100 bar), with the tri-layered neural network performing best for gravimetric capacity (R^2 = 1.00, RMSE = 0.237) and GPR for volumetric capacity (R^2 = 0.98, RMSE = 1.689). Their fine tree model showed superior generalization to unseen MOFs, with gravimetric uptake MSE 64.5% lower than ERT and 63.2% lower than GCMC simulations versus experimental data.

Additionally, the PCT curve serves as a crucial metric for evaluating the practical performance of hydrogen storage materials, and its accurate prediction holds significant importance for engineering applications. Kim et al. [38] employed a DNN model to predict the PCT behavior of AB_2 alloys at different temperatures, achieving an average correlation coefficient of 0.9307. This model accurately captures hysteresis phenomena and plateau pressure changes during hydrogen absorption/desorption processes, providing reliable basis for the engineering design of hydrogen storage systems. Zhou et al. [37] applied an SVM model to predict room-temperature equilibrium pressures of C14 Laves-phase alloys, obtaining a correlation coefficient above 0.97 with experimental data (Figs. 6(a–e)), demonstrating the advantages of ML in predicting complex thermodynamic behavior. Furthermore, a recent study [53] on NLi_4-BGra/MgH_2-based heterostructures integrated DFT

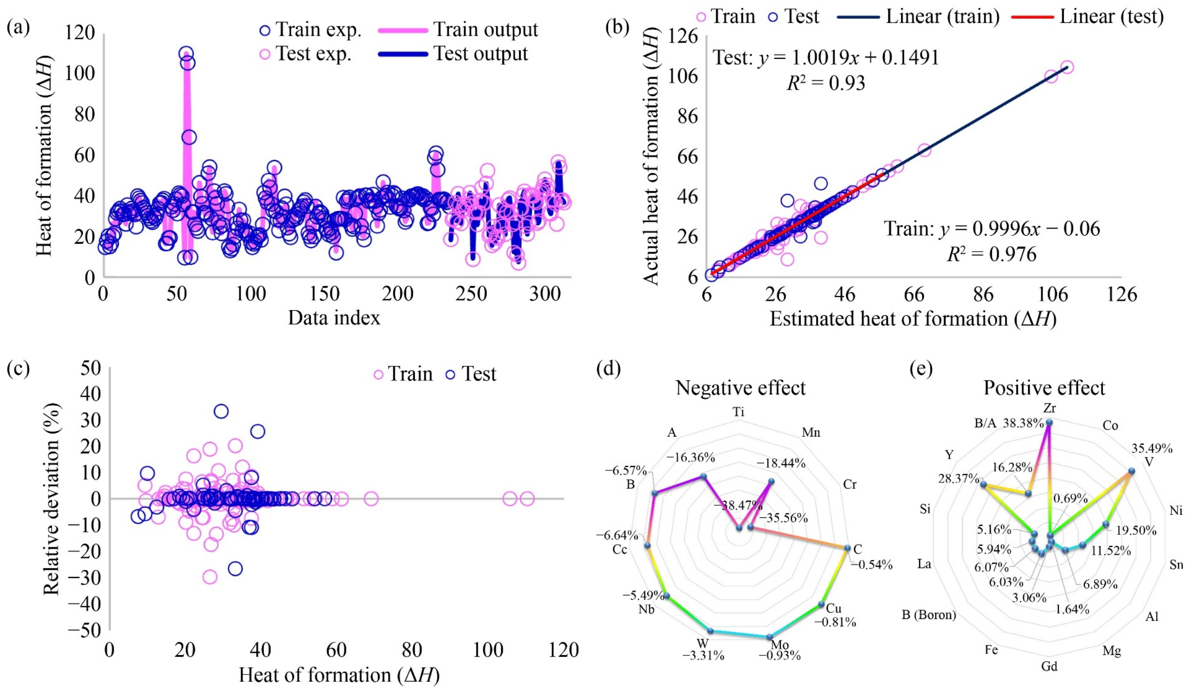

Fig. 5 Predictive behavior of GPR models using exponential kernel functions. (a) Comparison of actual and anticipated data for GPR model containing kernel function. (b) Cross plots for GPR model with kernel function. (c) Comparison of actual and anticipated data for GPR model containing kernel function. (d, e) Sensitivity analysis of the input variables for ΔH absorption of hydrogen on metal hydrides. Reprinted with permission from Ref. [52], copyright 2022, Springer Nature.

calculations with ML to predict dehydrogenation temperatures of 132 $MgMeH_x$ alloys, yielding a MAE of merely 26 K compared to DFT results. The work visualized the regulation of desorption temperature ranges via alloying (e.g., Li/Be doping) through Figs. 6(e) and 6(f), further validating ML's efficacy in predicting thermodynamic behaviors linked to PCT curve features for complex heterostructure systems.

Beyond thermodynamic properties, the kinetic characteristics and cycling stability of hydrogen storage materials are equally crucial. Ding et al. [56] employed an ensemble learning approach to predict the dehydrogenation kinetics of $LiBH_4$-based composites. Their ensemble model achieved a prediction accuracy of R^2 = 0.888, successfully identifying the key influencing factors, including factors such as catalyst type, dehydrogenation temperature, and heating rate. In the context of electrochemical hydrogen storage, Tian et al. [57] employed a BPNN to predict the cycle life of magnesium-based hydrogen storage alloys. Their model achieved an R^2 exceeding 0.99 for predicting the discharge capacity after the fifth cycle, thus providing a reliable tool for assessing material long-term stability.

These application cases demonstrate that ML models can now accurately predict key performance parameters of solid-state hydrogen storage materials across multiple dimensions, with prediction accuracy generally matching or even surpassing traditional empirical formulas and semi-empirical models. More importantly, these models operate 3–4 orders of magnitude faster than first-principles calculations, enabling large-scale material property evaluations and thus laying a solid foundation for subsequent high-throughput screening and new material discovery.

3.2 Current progress

3.2.1 Accelerated screening of new materials

The composition-structure space of solid-state hydrogen storage materials exhibits exponentially increasing complexity, rendering traditional experimental methods insufficient to effectively explore this vast space. The introduction of ML technology has fundamentally transformed the paradigm of materials discovery, enabling researchers to shift from experience-driven to data-driven approaches.

Building upon this paradigm shift, the integration of high-throughput computational screening (HTCS) and ML has emerged as a powerful approach for accelerating the exploration of vast material spaces [58]. HTCS enables systematic generation and evaluation of candidate compounds, while ML models capture complex, nonlinear correlations among composition, structure, and hydrogen storage performance. Together, they provide an efficient closed-loop workflow that can rapidly identify promising materials, reduce experimental trial-and-error, and guide data-driven design with predictive precision. To date, this synergistic strategy has been increasingly applied to diverse hydrogen storage systems, particularly

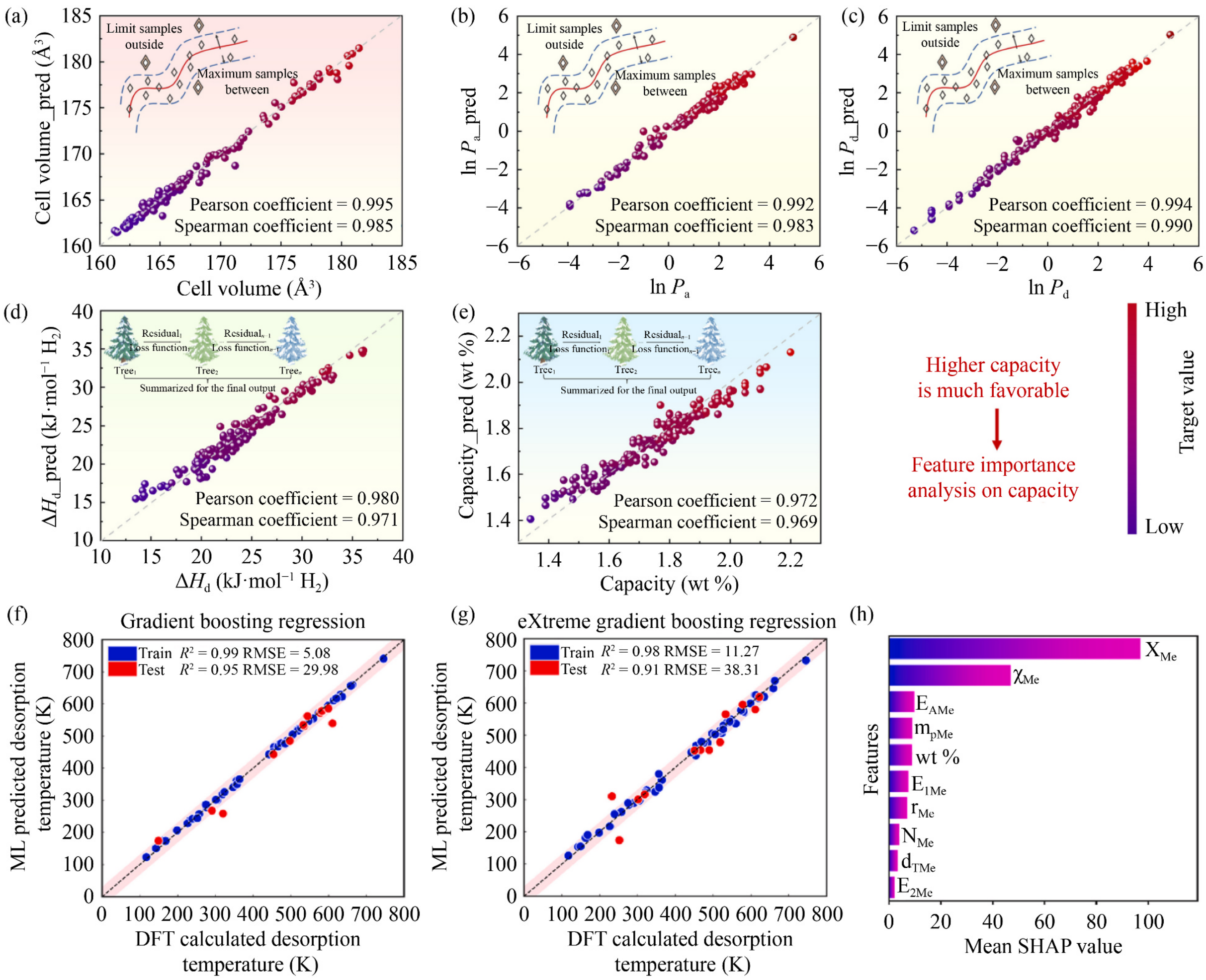

Fig. 6 (a–e) Demonstrate the predictive performance of ML models (SVM or gradient-boosted decision trees) optimized for key structural and hydrogen storage properties. Reprinted with permission from Ref. [37], copyright 2023, Elsevier. (f, g) Presents a ratio diagram of desorption temperatures for different tree models. (h) Indicates the evaluation of the feature SHAP. Reprinted with permission from Ref. [53], copyright 2024, Elsevier.

porous frameworks such as covalent organic frameworks (COFs) and MOFs [59]. Recent studies have demonstrated the effectiveness of this approach in improving both prediction accuracy and material discovery efficiency. Giappa et al. [60] integrated high-precision ab initio calculations with high-throughput GCMC simulations to evaluate functionalized benzenes and IRMOFs, identifying –OSO_3H as the most effective group for enhancing H_2 binding and uptake. Using 1138 *ab initio* data points, their ML models achieved chemical accuracy (–10^{-4} Ha), demonstrating that HTCS-generated atomic data can effectively guide ML-based functionalization design. Cao et al. [61] constructed an ionic liquid/COF database of 1398 samples using Monte Carlo simulations (CBMC and GCMC), then developed ML models for H_2 adsorption prediction, with CatBoost achieving the highest accuracy (R^2 = 0.9999, RMSE = 0.2628). The model enabled expansion to 6771 composites and identified [MMIM][Cl]@JUC-564 as a top-performing material (51.5 mmol·g^{-1} at 298 K and 100 bar). Feature analysis showed that pore volume, free volume, and density were dominant factors governing adsorption capacity. Similarly, Chen et al. [62] applied HT GCMC simulations to 2902 COFs and trained GBR and crystal graph CNN models. The GBR model achieved high accuracy (MAE = 0.061 wt % for gravimetric, 0.456 g·L^{-1} for volumetric capacity) and was used to screen over 95000 hypothetical COFs, revealing that Mg-alkoxide functionalization significantly enhances volumetric storage, especially in small-pore COFs. Overall, these findings collectively underscore the transformative potential of HTCS-ML frameworks in accelerating the discovery of hydrogen storage materials and expanding the accessible design space.

In this context, the construction of a virtual material space is a prerequisite for enabling high-throughput screening. Current high-throughput screening efforts are built upon the integration of multi-source data. The HydPARK data set, serving as a benchmark database in the field of hydrogen storage materials, contains experimental data for 2722 materials. However, a single data source alone struggles to meet the demands of large-scale screening. Nations et al. [51] innovatively merged the HydPARK data set with the Materials Project database, establishing a cross-scale screening platform. Using an RF ensemble model, they achieved rapid prediction of arbitrary hydrogenation energies (MSE = 0.102 eV^2), expanding the explorable material space from thousands of experimentally known compounds to tens of thousands of theoretically possible combinations. The key to this data fusion strategy lies in unifying the feature space. Researchers adopted the Magpie framework [63] as a universal feature descriptor, comprising 145 features covering stoichiometry, elemental properties, electronic structure, and ionization characteristics. This standardized feature representation enables the analysis and comparison of material data from diverse sources and types within a unified framework. Nonetheless, when confronted with the vast candidate material space, a hierarchical screening strategy has proven to be the most effective approach. The screening framework developed by Witman et al. [64] employs a three-tiered filtering mechanism. Tier 1 involves coarse screening coarse screening based on thermodynamic stability. A GBDT model rapidly evaluates the formation energies of 17920 isomolar HEAs, eliminating thermodynamically unstable combinations. This step can be completed within hours and incurs minimal computational cost. Tier 2 involves parallel evaluation of multiple performance metrics. For materials passing the initial screening, four key properties are simultaneously predicted: hydrogen storage capacity, hydride formation enthalpy, formation entropy, and equilibrium pressure (Fig. 7(a)). The model achieved the following prediction accuracy: MAE for hydrogen storage capacity = 0.14, MAE for formation enthalpy = 5.4 $kJ \cdot mol^{-1}$ H_2, MAE for formation entropy = 13 $J \cdot mol^{-1} \cdot K^{-1}$ H_2, and MAE for equilibrium pressure at 0 = 1.5. Tier 3 involves application-scenario-based fine-tuning. Additional constraints are applied based on specific application requirements (e.g., vehicle hydrogen storage, stationary energy storage), including operating temperature ranges, pressure windows, and cost limitations.

Building upon this foundation, the incorporation of active learning and multi-objective optimization strategies has introduced new levels of efficiency and accuracy to the screening process. Active learning dynamically selects the most representative or promising data points for supplementary computation through uncertainty sampling, enabling the model to continuously optimize performance even under limited sample conditions, thereby reducing computational overhead. Furthermore, hydrogen storage material design inherently involves a multi-objective optimization problem, with complex trade-offs among various performance metrics. The Pareto optimization approach adopted by Witman et al. [64] offers a systematic solution. By constructing a four-dimensional Pareto frontier, researchers can identify material combinations achieving an optimal balance across multiple objectives, including hydrogen storage capacity, thermodynamic stability, kinetic performance, and cost-effectiveness, as shown in Figs. 7(b) and 7(c).

On the other hand, reverse design methodologies are gradually demonstrating promising applications. Unlike traditional forward prediction, which derives properties from composition, reverse design approaches start from performance requirements. Through ML models or generative algorithms, they reverse-engineer potential material compositions and structures, thus enabling goal-driven material development. Hattrick-Simpers et al. [65] combined techno-economic analysis to identify materials suitable for hydrogen compressors from a pool of 6110 potential alloys. By imposing constraints on cost, composition, and potential structure, they ultimately narrowed the candidate materials to fewer than 400, identifying the Fe-Mn-Ti-X alloy system as an ideal candidate. Lee et al. [66] applied GANs to design two-dimensional MgH_2 layered materials, achieving a 96.8%

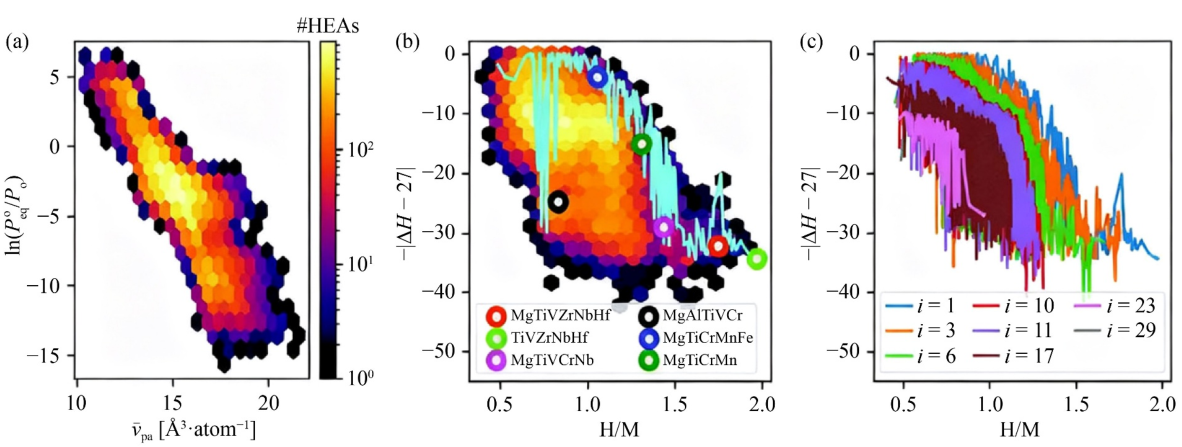

Fig. 7 (a) Predicted equilibrium pressure based on screening of 17920 special isothermal high-energy alloys with $\bar{v}_{pa}$; (b) projection of the four-dimensional Pareto frontier onto a two-dimensional plot; (c) evolution process of the i-th Pareto frontier material after removing the (i-1)-th Pareto frontier material. Reprinted with permission from Ref. [64], copyright 2023, Royal Society of Chemistry.

structure validation rate and an 87.3% structure generation rate. This approach successfully discovered novel two-dimensional MgH_2 phases belonging to the $P\bar{4}m2$ space group, thereby opening new avenues for innovative hydrogen storage material design. Unlike most studies focusing only on predictive modeling, Lu et al. [44] introduced FIND (Forward-Inverse Navigation and Discovery), a data-driven platform for hydrogen storage alloys (Fig. 8(a)). Beyond forward prediction, it uses a variational autoencoder (VAE) for inverse design

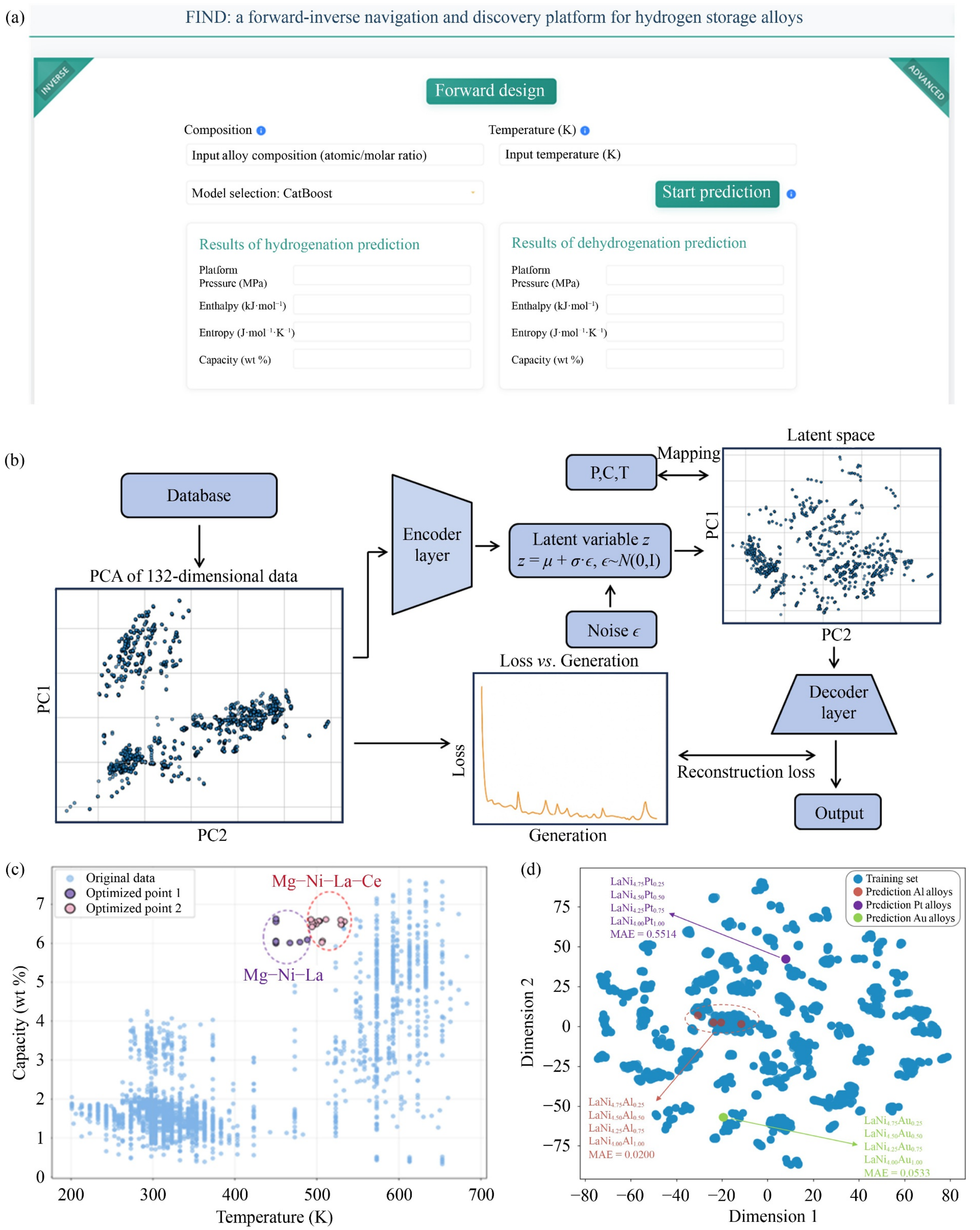

Fig. 8 (a) Homepage of the FIND platform. (b) Inverse discovery framework for hydrogen storage alloy design on the FIND platform. (c) Distribution of the potential optimal alloys in the original database. (d) t-SNE dimensionality reduction distribution of $LaNi_{5-x}M_x$ (M = Al, Pt, Au, x = 0.25, 0.50, 0.75, 1.00) alloys in the original database at 298 K. Reprinted with permission from Ref. [44], copyright 2025, the Author(s).

(Fig. 8(b)), generating candidate alloys directly from targetproperties.Combinedwithgenetic-algorithmoptimization, FIND identified 27 promising Mg-Ni-La-Ce alloys with dehydrogenation temperatures of 450–533.5 K, expanding the accessible performance range (Fig. 8(c)). Reliability checks ensured physical plausibility, and dimensionality reduction revealed meaningful structural distributions. As shown in Fig. 8(d), the t-distributed stochastic neighbor embedding (t-SNE) projection of $LaNi_{5-x}M_x$ alloys (M = Al, Pt, Au; x = 0.25–1.00) at 298 K displays distinct clusters, with Al-doped alloys in dense training regions and low prediction errors (MAE = 0.0200), while Pt- and Au-doped alloys form separate clusters with larger errors (Pt MAE = 0.5514, Au MAE = 0.0533). Overall, FIND demonstrates a reusable, platform-oriented workflow for accelerating hydrogen storage alloy discovery.

In summary, ML has progressively shifted the screening approach for solid-state hydrogen storage materials from experience-driven methods to data-driven strategies. The integration of virtual material space, active learning, multi-objective optimization, and inverse design is establishing a new intelligent closed-loop paradigm for materials design. This transformation not only accelerates the discovery of potential materials but also provides a solid foundation for the future development of fully automated materials discovery platforms.

3.2.2 High-throughput computing integration

In solid-state hydrogen storage material research, insufficient data scale and quality have long been key bottlenecks limiting ML model performance. While traditional experiments and DFT calculations can deliver high-precision results, they prove significantly inefficient when confronting the vast chemical space of materials. The introduction of high-throughput computing offers a solution to this challenge. By systematically generating large-scale, consistent data across the material combination space, it not only provides high-quality training inputs for ML models but also establishes a robust foundation ensuring the physical plausibility of predictive outcomes. This approach has evolved into the research paradigm of high-throughput computing integrated with ML, driving the transition of solid-state hydrogen storage materials from experience-driven to intelligence-driven development.

In the field of HEAs, Somo et al. [48] systematically demonstrated the advantages of combining high-throughput computing with ML, with the workflow illustrated in Fig. 9. They constructed a database covering 304 HEA compounds using DFT-based high-throughput calculations, incorporating key performance parameters such as hydrogenation enthalpy, hydrogen/metal ratio, and equilibrium temperature. Building on this foundation, the authors trained multiple ML models and found that RF delivered the best performance after integrating high-throughput DFT data, achieving prediction accuracy with R^2 values close to 0.93–0.95. More importantly, feature importance analysis identified valence electron concentration (VEC) as the core factor determining the thermodynamic hydrogen storage performance of HEAs, a qualitative pattern highly consistent with experimental trends. This research not only enhances prediction efficiency but also demonstrates that systematic data from high-throughput computations can strengthen a model's physical plausibility, thus avoiding the 'black-box' dilemma inherent in purely data-driven approaches.

In complex hydride systems, high-throughput computation also demonstrates its unique value. Jia et al. [67] used $Mg(BH_4)_2$ as a model system, integrating 5832 experimental/computational data points from over 70 literature sources and computational simulations to construct a large-scale database supporting subsequent

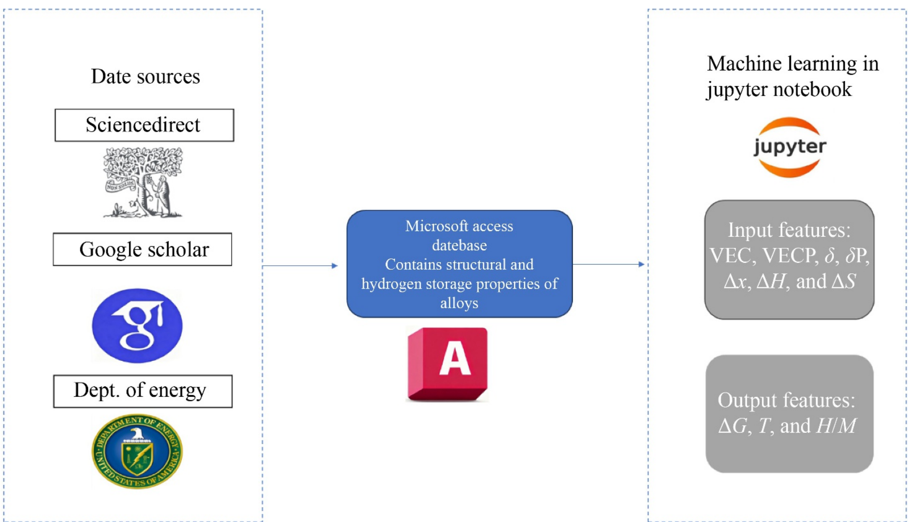

Fig. 9 Schematic diagram of the data collection and ML process. Reprinted with permission from Ref. [48], copyright 2025, Elsevier.

ML model training, with the workflow illustrated in Fig. 10. They proposed a multi-head attention mechanism neural network model that outperformed traditional algorithms like SVM and RF in predicting both isothermal and non-isothermal dehydrogenation processes. More notably, this model revealed key variable thresholds governing dehydrogenation behavior, including temperature windows, impurity content, and crystal structure factors, through interpretable analysis of attention weights. Building on these findings, the authors experimentally synthesized the $Mg(BH_4)_2$-$LiBH_4$-FGi composite system and validated the model's prediction of highly efficient dehydrogenation performance. This case vividly demonstrates that integrating high-throughput databases with advanced ML methods not only enables high-precision predictions in virtual space but also directly guides experimental parameter optimization through interpretable mechanisms, forming a closed-loop system integrating theory, modeling, and experiment.

From a broader perspective, Zhou et al. [49] emphasize that high-throughput computation is a critical component for overcoming ML bottlenecks. Its value lies not only in generating large-scale data sets but also in ensuring data comparability and reliability through standardized protocols and automated workflows. They point out that future trends will involve the tight integration of high-throughput computation, active learning, and experimental validation to construct consistent databases across material systems, thereby overcoming current limitations due to sparse and unevenly distributed data. For instance, active learning strategies can dynamically select new sampling points for high-throughput computation based on model prediction uncertainty, maximizing model accuracy gains while minimizing computational cost.

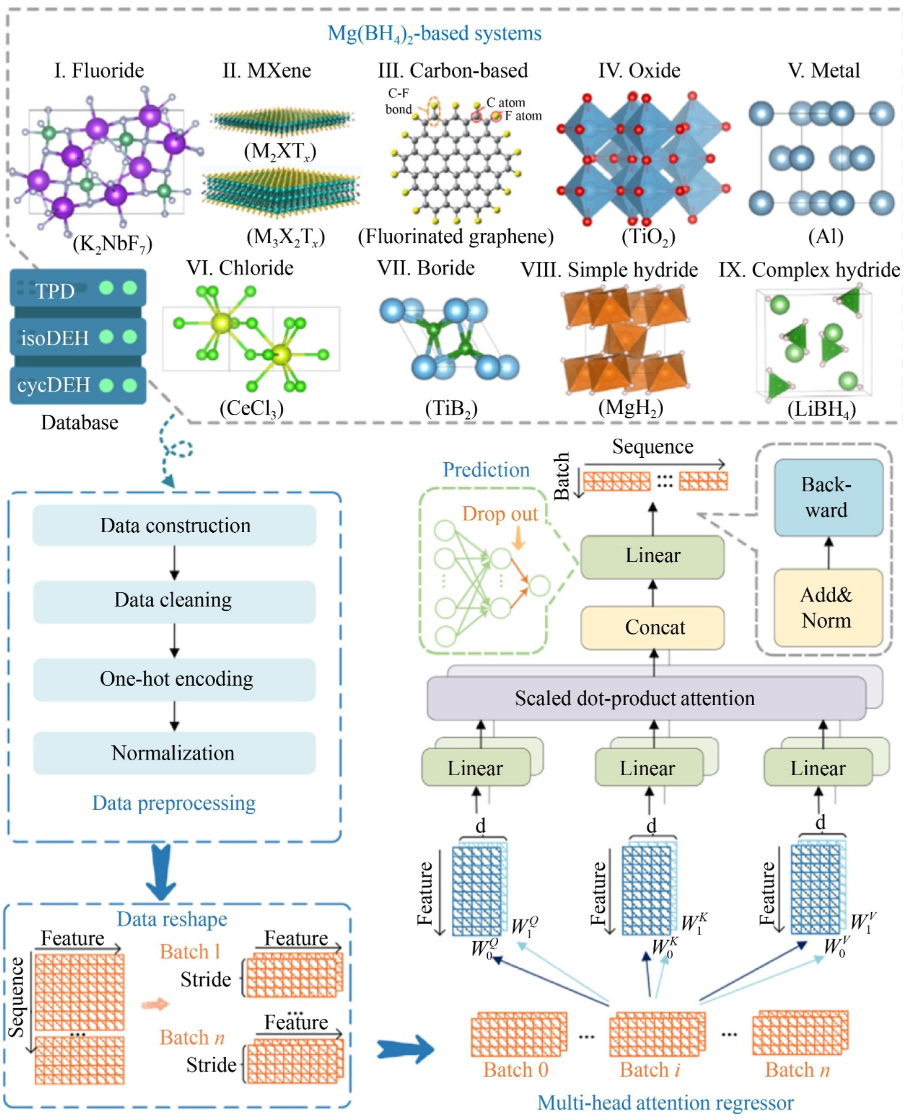

Fig. 10 Flowchart of the SC data set classification process and a schematic diagram of the MAR neural network model's processing steps. Reprinted with permission from Ref. [67], copyright 2025, National Engineering Research Center for Magnesium Alloys of China, Chongqing University.

This dynamic data acquisition approach propels ML from static training toward self-evolving paradigms, significantly enhancing its extrapolation capabilities in unknown systems.

In summary, the integration of high-throughput computing and ML is emerging as a core driving force in solid-state hydrogen storage material research. Within the HEAs framework, it reveals hydrogen storage mechanisms through systematic databases and feature identification; in complex hydrides, it integrates performance prediction with experimental guidance by combining large-scale data and deep learning; and in overall methodology, it propels a paradigm shift from static modeling to dynamic adaptation. With the continuous expansion of computational resources and ongoing optimization of algorithmic methods, the integration of high-throughput computing is poised to further advance solid-state hydrogen storage material research toward comprehensive intelligence and automation, providing robust support for the rapid design and discovery of future novel materials.

3.2.3 Emerging AI paradigms

Beyond conventional ML models and predictive platforms, recent advances have heralded a new paradigm in solid-state hydrogen storage research: the integration of large language models (LLMs) and AI agents. Specifically, these developments highlight a shift from purely model-driven approaches to intelligent, multi-agent systems that are not only capable of autonomous data acquisition and reasoning but also facilitate more efficient materials design.

A representative example is Yao et al. [68]'s 'LLM-to-Agent' framework for MgH_2 dehydrogenation catalyst design. The study established an end-to-end workflow (Fig. 11(a)) that integrates LLM-based literature extraction, machine-learning prediction of key performance indicators, and genetic-algorithm inverse design. Applied to 759 publications, the pipeline produced 2360 validated entries covering 809 catalysts and 6555 structure-property records, yielding an approximately fortyfold increase in data curation efficiency relative to manual extraction (Fig. 11(b)). The curated data set not only supported automated statistical analyses of catalyst performance (Fig. 11(c)) but also enabled training of high-accuracy ML models for onset dehydrogenation temperature and activation energy. Subsequently, these models guided a genetic-algorithm search that identified clusters of previously unexplored, high-performance candidates (Fig. 11(d)). Finally, Cat-Advisor, a domain-adapted multi-agent system that integrates retrieval-augmented knowledge with ML outputs, outperformed general-purpose LLMs in domain benchmarks and now provides interactive, domain-specific design assistance. In parallel, Zhang et al. [69] introduced the DIVE (descriptive interpretation of visual expression) workflow, which leverages multi-agent orchestration to extract structured data directly from complex graphical elements in the literature. Applied to over 4000 publications on solid-state hydrogen storage materials, DIVE achieved 10%–15% accuracy gains over commercial multimodal models and over 30% improvements relative to open-source models. The resulting curated database of more than 30000 entries enabled the development of DigHyd, an AI agent capable of performing rapid inverse design and generating novel candidate compositions within minutes.

Collectively, these studies exemplify the emerging role of AI agents in bridging unstructured knowledge with structured predictive modeling, thereby transforming hydrogen storage research from data scarcity to interactive, agent-driven discovery. Rather than isolated tools, they mark the transition toward integrated ecosystems where AI agents may increasingly act as collaborative partners in autonomous materials discovery, with the potential to interface seamlessly with both data platforms and experimental laboratories.

3.3 Challenges and shortcomings

As previously mentioned, ML in the field of solid-state hydrogen storage remains underdeveloped, with its primary challenges and shortcomings including limited database quality and scale, as well as the trade-off between model interpretability and accuracy. The following sections will elaborate on these challenges individually and propose corresponding solution strategies.

3.3.1 Poor database quality and scale

Acquiring performance data for solid-state hydrogen storage materials is costly and particularly time-consuming, resulting in a severe shortage of high-quality data sets. Although the current HydPARK database encompasses most solid-state hydrogen storage system data, data quality issues persist, including duplication, missing entries, limited data set size, and inaccuracies. Researchers have addressed this by cleaning, filtering, and refining the database to produce multiple improved versions. Nevertheless, the data volume and quality for specific material systems remain insufficient to meet the demands of robust ML applications [70]. Meanwhile, the thermodynamic properties of hydrogen storage materials are primarily governed by intrinsic factors such as elemental composition, crystal structure, grain size, atomic occupancy, and stoichiometry. Despite identical compositions and structures, materials often exhibit significant performance variations across different laboratories. This discrepancy stems mainly from external factors, including preparation processes, testing conditions (temperature, pressure), instrument precision

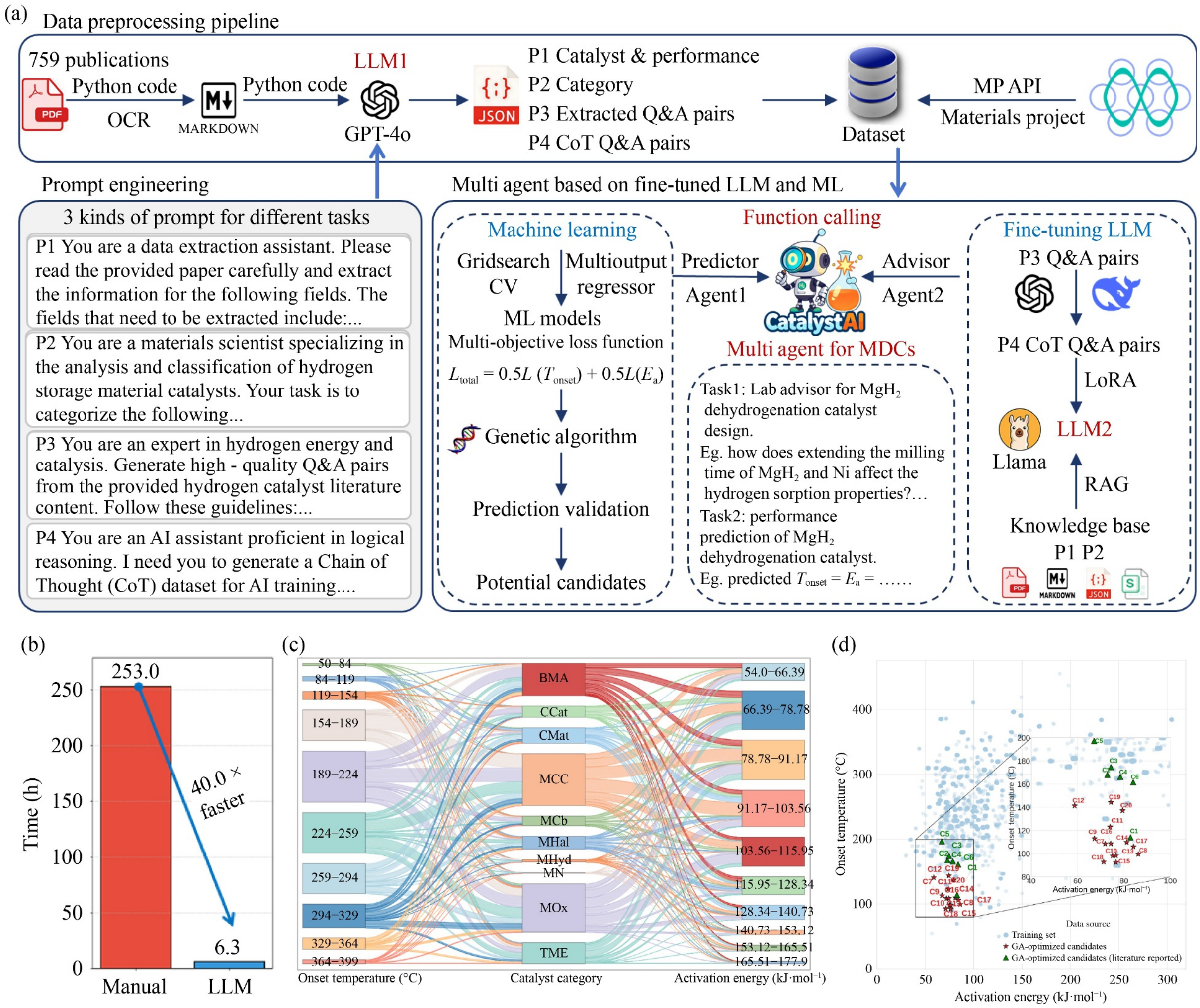

Fig. 11 (a) Schematic of an LLM-driven ML framework for MgH_2 dehydrogenation catalyst design. (b) Comparison of the automated pipeline method *vs*. average manual execution time for 759 publications. (c) Sankey diagram of catalyst material categories, onset dehydrogenation temperature (T_{onset}), and activation energy (E_a). (d) Performance landscape plot comparing the distribution of the top 20 GA-identified candidates against the training set, demonstrating the successful identification of a high-performance solution cluster by the GA. Reprinted with permission from Ref. [68], copyright National Engineering Research Center for Magnesium Alloys of China, Chongqing University.

(volume measurement, sensor sensitivity, and hydrogen purity), and hydrogen storage device design. Such inconsistencies in experimental data directly limit the predictive accuracy and generalization capability of ML models.

From a data perspective, both high-performance and low-performance data points play equally important roles in shaping the generalization capability of ML models [23,71]. Each data point contributes to defining the overall feature-property landscape, enabling the model to capture comprehensive correlations across the performance spectrum. However, given the data inconsistencies discussed above, ensuring data quality through rigorous inspection and preprocessing is indispensable before model training. Outliers arising from experimental errors, measurement inconsistencies, or inaccurate reporting can introduce bias and degrade model accuracy. Therefore, the careful identification and removal of anomalous data points represent a crucial step in eliminating unreliable information and enhancing data reliability [72]. For instance, Wilson et al. [73] developed the HyStor database by expanding and curating the HydPARK data set, in which they identified and corrected duplicate, conflicting, and erroneous records, and flagged unrepresentative outliers through multiple validation tests. At the same time, they retained low-performing yet physically meaningful samples to preserve data set diversity, ensuring that models could learn balanced correlations across the entire performance range. As a result of this targeted refinement, the model's MAE decreased from 0.31 to 0.29, and the R^2 score improved from 0.77 to 0.79.

Academic and industrial communities have proposed multiple strategies to address systemic issues related to data quality and availability in solid-state hydrogen storage materials. These strategies mainly focus on constructing high-quality databases, applying intelligent data mining techniques, and leveraging transfer learning and supervised learning methods.

In terms of database standardization, establishing a shared hydrogen storage materials database is considered the fundamental solution to address data fragmentation and inconsistencies in quality. This process requires developing uniform data standards and format specifications covering material composition, structural parameters, preparation techniques, testing conditions, and performance metrics. By implementing standardized protocols for data collection, storage, and sharing, disparities between research institutions can be effectively minimized, thereby enhancing data comparability and reliability. Meanwhile, the advancement of intelligent data mining technologies offers new solutions to overcome traditional data acquisition bottlenecks. Literature mining techniques based on natural language processing and LLMs can automatically extract structured data from vast scientific literature, significantly enhancing data collection efficiency [34]. The Python automation tool developed by Huang et al. [34] demonstrates the immense potential of this technical approach. This tool not only enables batch downloading and processing of literature but also accurately identifies and extracts key information, including chemical formulas, reaction conditions, and performance parameters, through deep learning algorithms. Compared to traditional manual data curation methods, this approach exhibits significant advantages in both efficiency and accuracy. The tool's application scope covers major hydrogen storage material systems, including magnesium-based, aluminum-based, boron-based, and nitrogen-based materials, successfully constructing a comprehensive data set containing over 2000 entries. More importantly, through deep integration with existing materials genome databases (such as the Materials Project, the Open Quantum Materials Database, and Automatic-FLOW for Materials Discovery Library), researchers obtained detailed information on 6468 hydrogen-containing materials. This data set encompasses seven crystal systems, 187 space groups, and 8118 distinct crystal structure types, and includes key physicochemical parameters such as composition, oxidation states, bond lengths, and bond angles.

Transfer learning techniques demonstrate significant technical advantages in hydrogen storage material research. By leveraging pre-trained models from related domains, transfer learning effectively addresses the challenge of insufficient training data in target domains, substantially enhancing both model prediction accuracy and generalization performance for novel material systems. In practical applications, Batalovic et al. [74] developed a transfer learning framework based on material graph networks specifically for predicting the hydride formation enthalpy of magnesium-based hydrogen storage materials. This framework utilizes crystal structure information of intermetallic compounds as input and successfully delivers high-precision thermodynamic property predictions by transferring feature representations and learning strategies from pre-trained models.

Furthermore, unsupervised and semi-supervised learning methods hold significant application value in scenarios with scarce hydrogen storage material data. Unsupervised learning can uncover intrinsic structures and latent patterns within data despite the absence of labeled information, offering novel perspectives for material property analysis. Meanwhile, semi-supervised learning techniques effectively mitigate the challenges of high labeling costs and insufficient data by integrating small amounts of labeled data with large volumes of unlabeled data for collaborative training [75]. Applications of semi-supervised learning in materials science have demonstrated promising outcomes. The semi-supervised learning framework developed by Chen et al. [76] provides an effective paradigm for microstructural analysis. Based on the U-Net architecture, this method achieves high-precision microstructural segmentation using only a small number of labeled samples through adaptive learning strategies and an improved pseudo-label selection mechanism. These findings highlight the ability of semi-supervised learning to reduce reliance on manual labeling while enhancing model generalization performance. For solid-state hydrogen storage materials research, these methods can fully leverage vast amounts of unlabeled experimental data and theoretical computational results. By uncovering latent correlations within the data, they significantly enhance model prediction accuracy and robustness. Particularly in the exploration of new material systems and performance optimization, semi-supervised learning techniques hold considerable promise for accelerating hydrogen storage material R&D and reducing experimental validation costs.

Beyond the above strategies, interactive visual analytics tools have emerged as a valuable complement. Shao et al. [77] developed the FAIR (feature-space analysis and insight for reliability) platform, an open-source tool designed to identify and mitigate 'data unfairness', including data set imbalance, sparsity, and unsafe extrapolation. FAIR transforms high-dimensional feature spaces into intuitive visualizations (via PCA, t-SNE, and uniform manifold approximation and projection), allowing researchers to detect and address data defects directly. Its redundancy-reduced sampling can cut data set size by over 60% while retaining essential information, and its exploration-based sampling adds targeted data to fill sparse regions, reducing MAE by over 80% in sparse data sets. Additionally, the credibility analysis toolkit quantifies distribution mismatches and flags high-risk extrapolation scenarios. This human-in-the-loop approach improves prediction reliability even with low-quality or limited data sets, addressing inaccuracies caused by data defects.

3.3.2 Compatibility of model interpretability and high accuracy

In the field of solid-state hydrogen storage materials research, a significant tension exists between the predictive accuracy of ML models and their interpretability. Complex ensemble learning and deep learning models, including GBR, extreme gradient boosting, and DNNs, can achieve exceptionally high prediction accuracy on training data sets [34]. However, they often exhibit ‘black-box’ characteristics, failing to reveal the underlying physical principles behind their predictions. In the context of materials science research, high prediction accuracy alone is insufficient. Researchers seek models that reveal key descriptors, microscopic mechanisms, and causal relationships between composition, structure, and properties, thereby providing guidance for both experimental and theoretical advancements.

Existing research clearly highlights this contradiction. For instance, Somo et al. [48] combined DFT with RF models to predict the hydrogenation enthalpy and equilibrium temperature of HEAs, achieving high accuracy with R^2 values ranging from 0.90 to 0.95. However, the extrapolation capability and reliability of their predictions still require confirmation through experimental validation and feature importance analysis. Dangwal et al. [26] predicted hydrogenation enthalpy for HEAs using GPR, achieving high consistency with DFT and experimental results. This demonstrates that for specific systems, models can balance accuracy with partial interpretability, though its generalizability remains constrained by training data scale. Similarly, Radhika et al. [78] employed multiple ML models to predict hydrogen-to-metal ratios (H/M) and VEC, successfully proposing 774 potential HEA candidates. However, the study itself acknowledges that insufficient interpretability continues to remain a primary obstacle limiting the practical application of these results. In the field of porous materials, Kim et al. [27] employed ML to screen MOFs, successfully synthesizing novel V-based MOFs, achieving 9.0 wt % hydrogen storage capacity. Nevertheless, the authors noted that although the model predictions were accurate, they could not directly reveal the fundamental causal relationship between pore structure and hydrogen storage behavior.

To address this issue, researchers have proposed various improvement methods. One approach combines post-processing interpretability techniques, such as SHAP and LIME (local interpretable model-agnostic explanations), to quantify the contribution of different features to prediction outcomes, thereby enhancing model transparency without compromising accuracy. For instance, Yang et al. [79] employed a GBDT algorithm with high accuracy. By conducting feature importance analysis, they demonstrated the decisive influence of bandgap parameters on the dielectric properties of polycrystalline materials, providing quantitative insights into the correlation between microstructure and macroscopic electrical properties. Zhou et al. [37] conducted a systematic analysis of C14-type alloys using the SHAP interpretability method. Their results indicate a clear negative correlation between the iron content in the alloy and the material’s hydrogen storage capacity, with model predictions suggesting that the hydrogenation equilibrium pressure could reach gigapascal levels under room temperature conditions.

Another approach involves developing physically constrained ML models, which explicitly incorporate known thermodynamic or electronic structure principles during training, thereby preventing the models from deviating from physical reality while maintaining numerical accuracy. Additionally, a hybrid modeling approach has emerged, effectively balancing the trade-off between predictive performance and interpretability by integrating the strengths of different algorithms. The core idea of this strategy is to leverage high-performance yet complex algorithms for feature learning tasks, followed by applying more transparent models for final predictions, enhancing model interpretability while maintaining predictive accuracy.

3.3.3 Limitations of the design methodology

Although ML has significantly accelerated the screening and performance prediction of solid-state hydrogen storage materials, notable limitations persist at the level of design methodology.

First, current research primarily focuses on forward prediction, which infers hydrogen storage performance from material composition and structure. While such methods enhance screening efficiency, they remain fundamentally ‘performance evaluation tools’ rather than ‘performance-driven generation tools’. The absence of reverse design approaches severely constrains ML’s innovative potential in materials discovery. Some studies attempt to mitigate this by expanding the search space. For instance, Radhika et al. [78] proposed 774 potential HEA hydrogen storage candidates, while Gao et al. [80] built predictive models based on 918734 MOFs data points to screen 8282 high-capacity candidates. Nevertheless, these approaches still follow the predict-screen-synthesize paradigm, essentially identifying promising candidates from vast material libraries rather than directly generating novel structures based on performance targets. Consequently, the absence of reverse design prevents ML from becoming the core engine driving original material discovery.

Second, existing models exhibit significant shortcomings in multiscale modeling. Solid-state hydrogen storage performance is influenced by the coupled effects of multiple hierarchical factors, including electronic structure, point defects, microstructure, and macroscopic transport properties. Yet most current ML models focus solely on a single hierarchical level. For instance, in MOF hydrogen storage research, Kim et al. [27] and Gao et al. [80] employed small-scale experimental data and a million-entry structure library for predictions, respectively. While these approaches effectively identified promising candidates, they did not adequately account for cross-scale effects such as pore structure evolution, defect influences, and synthesis conditions. Similarly, in the $Mg(BH_4)_2$ system, Jia et al. [67] proposed a neural network model based on multi-head attention mechanisms and revealed key variable thresholds through interpretability analysis. However, their research remains confined to a specific system and experimental parameter optimization, without achieving universal cross-scale inverse design.

In summary, current design methods exhibit three primary limitations: dominance of forward prediction with insufficient generative capability; absence of inverse design with inadequate goal-driven orientation; and lack of multiscale modeling hindering comprehensive characterization of complex hydrogen storage behavior. Future advancements require integrating advanced generative models such as reinforcement learning, generative adversarial networks, and VAEs to transition from ‘prediction’ to ‘creation’. Concurrently, cross-scale fusion approaches should be explored to unify electronic structure calculations, microscopic dynamics, and macroscopic heat transfer behavior within a ML framework, enabling more universal and actionable solid-state hydrogen storage material design.

4 NNPs for mechanistic understanding

4.1 NNPs for solid-state hydrogen storage: principles, advantages, and feasibility

The solid-state hydrogen storage process inherently involves the adsorption and dissociation of hydrogen molecules, the penetration of hydrogen atoms into the bulk material, and their diffusion and long-range migration within lattice interstices. Consequently, these coupled phenomena unfold across multiple temporal and spatial scales, encompassing both the breaking and formation of chemical bonds at the electronic-structure level and the cooperative motion of large numbers of atoms. For DFT, while it can accurately characterize the energy barriers of elementary steps and the associated electronic structure features, the computational cost becomes prohibitive for long-time dynamics or large-scale models [81,82]. Traditional empirical potentials are advantageous in terms of efficiency; however, their reliance on predefined functional forms and limited parameterization often result in insufficient accuracy under complex chemical environments such as hydrogen molecule dissociation or metal hydride phase transitions [83]. Against this backdrop, NNPs have emerged as a rational and efficient tool for investigating hydrogen storage and release mechanisms [84,85].

NNPs are designed to approximate the potential energy surface (PES) of atomic systems using ML techniques, thereby achieving near–first-principles accuracy at a fraction of the computational cost [86]. The basic concept involves using ab initio (typically DFT) energy-force data sets (sometimes also including stress) as the ‘teacher’, enabling the neural network to learn the nonlinear mapping between atomic local environments and their associated energies, ultimately yielding an approximate PES that can be applied to large systems over extended timescales [87−89].

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4.2 Current progress and applications

4.2.1 NNP-enabled surface H_2 interactions: adsorption dissociation and diffusion

Ludwig et al. [90] introduced a two-step NNP workflow, first, apply a corrugation-reducing procedure to smooth the metal surface and fit only the residual energy with a neural network; secondly, use novelty-driven sampling to couple molecular dynamics (MD) with an ab initio database until dynamical observables converge. Validated on analytical LEPS models and then on PW91-DFT for H_2/Pt(111), this offers an efficient, convergence-verifiable route to build 6D PESs for elementary surface reactions

Using an EANN trained on optPBE-vdW energies/forces, Zhu et al. [91] built a unified PES that includes surface degrees of freedom and validated it via quasi-

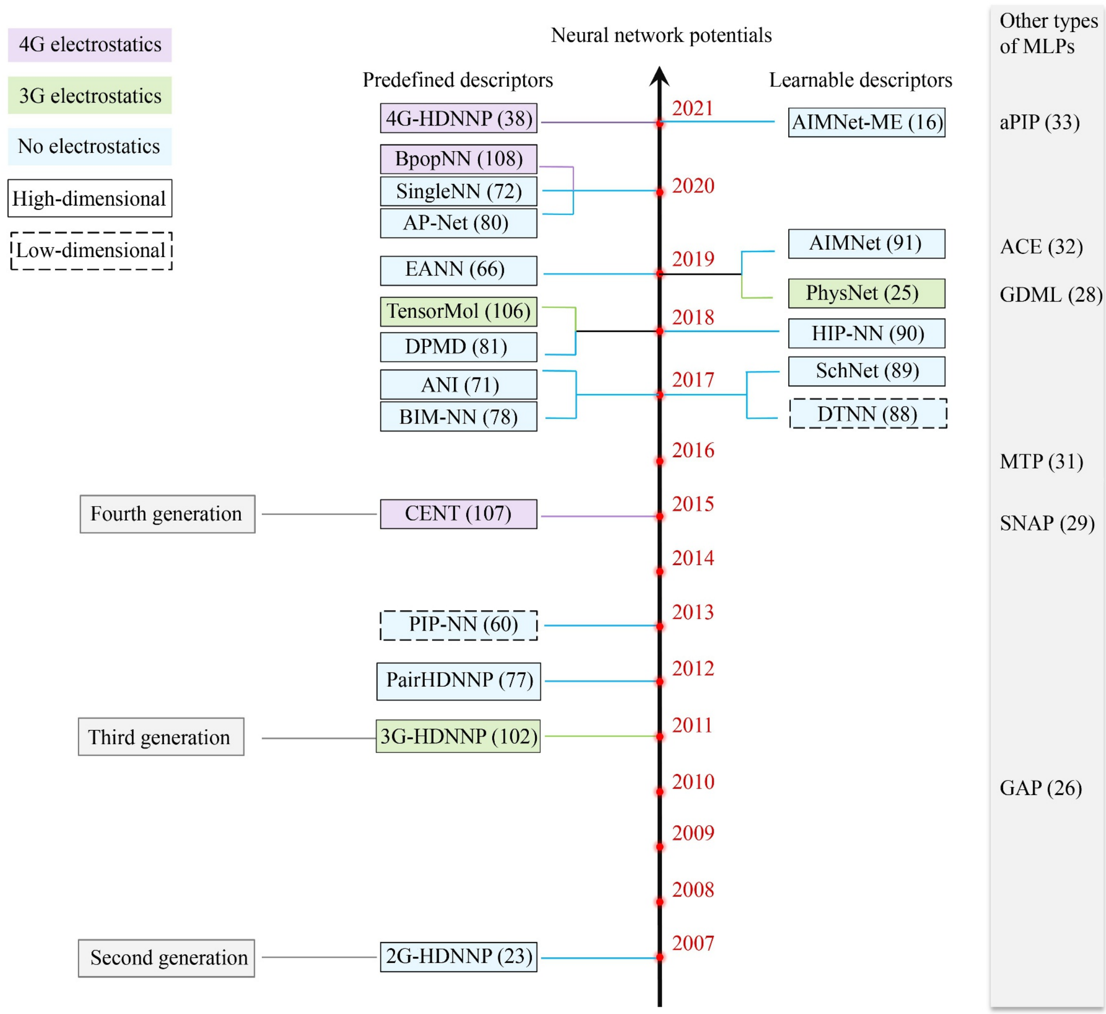

Fig. 12 Timeline for the evolution of NNPs. NNPs using predefined descriptors are shown on the left, and NNPs with learnable descriptors (message passing neural networks) are shown on the right. The frame width and background color label the dimensionality and the absence or inclusion of long-range electrostatic interactions in 3G and 4G potentials (abbreviations: ACE, atomic cluster expansion; AP-Net, atomic-pairwise neural network; aPIP, atomic permutationally invariant polynomial; BIM-NN, bonds-in-molecule neural network; BpopNN, Becke population neural network; CENT, charge equilibration via neural network technique; DPMD, deep potential molecular dynamics; DTNN, deep tensor neural network; EANN, embedded atom neural network; GAP, Gaussian approximation potential; GDML, gradient domain ML; HDNNP, high-dimensional NNP; HIP NN, hierarchically interacting particle neural network; MLP, machine learning potential; MTP, moment tensor potential; PIP-NN, permutation invariant polynomial neural network; SNAP, spectral neighbor analysis potential). Reprinted with permission from Ref. [87], copyright 2022, Annual Reviews.

classical trajectory (QCT) simulations with quantum dynamics cross-checks. QCT delivers ~10^5 × *ab initio* molecular dynamics (AIMD) speed-ups while reproducing H_2/D_2 dissociation/adsorption on Cu facets (and temperature effects), outlining a scalable, experiment-consistent pathway to model more complex, realistic surfaces. To accurately and robustly predict H_2 dissociative sticking and associative desorption under conditions involving multiple facets and explicit surface-atom motion, Stark et al. [92] developed a machine-learning interatomic potential for H_2 gas-solid scattering on multifaceted copper by combining E(3)-equivariant message-passing neural networks (e.g., PaiNN) with uncertainty-driven active sampling (Fig. 13(a)). A three-member committee was trained, using the standard deviation of predicted energies and forces as the acquisition criterion to iteratively augment the SRP48-DFT reference set. Convergence and cross-model consistency were assessed via sticking-probability versus incident-energy curves, and the dynamics employed large-ensemble quasi-classical scattering with explicit surface degrees of freedom. Relative to the non-equivariant SchNet baseline, the equivariant models achieved higher data efficiency, smoother PESs, and lower energy/force errors. The resulting 0 K sticking curves and ~925 K results for Cu(211)/Cu(111) exhibit improved agreement with experiment and prior theory, alongside reduced predictive uncertainty (Figs. 13(b–e)).

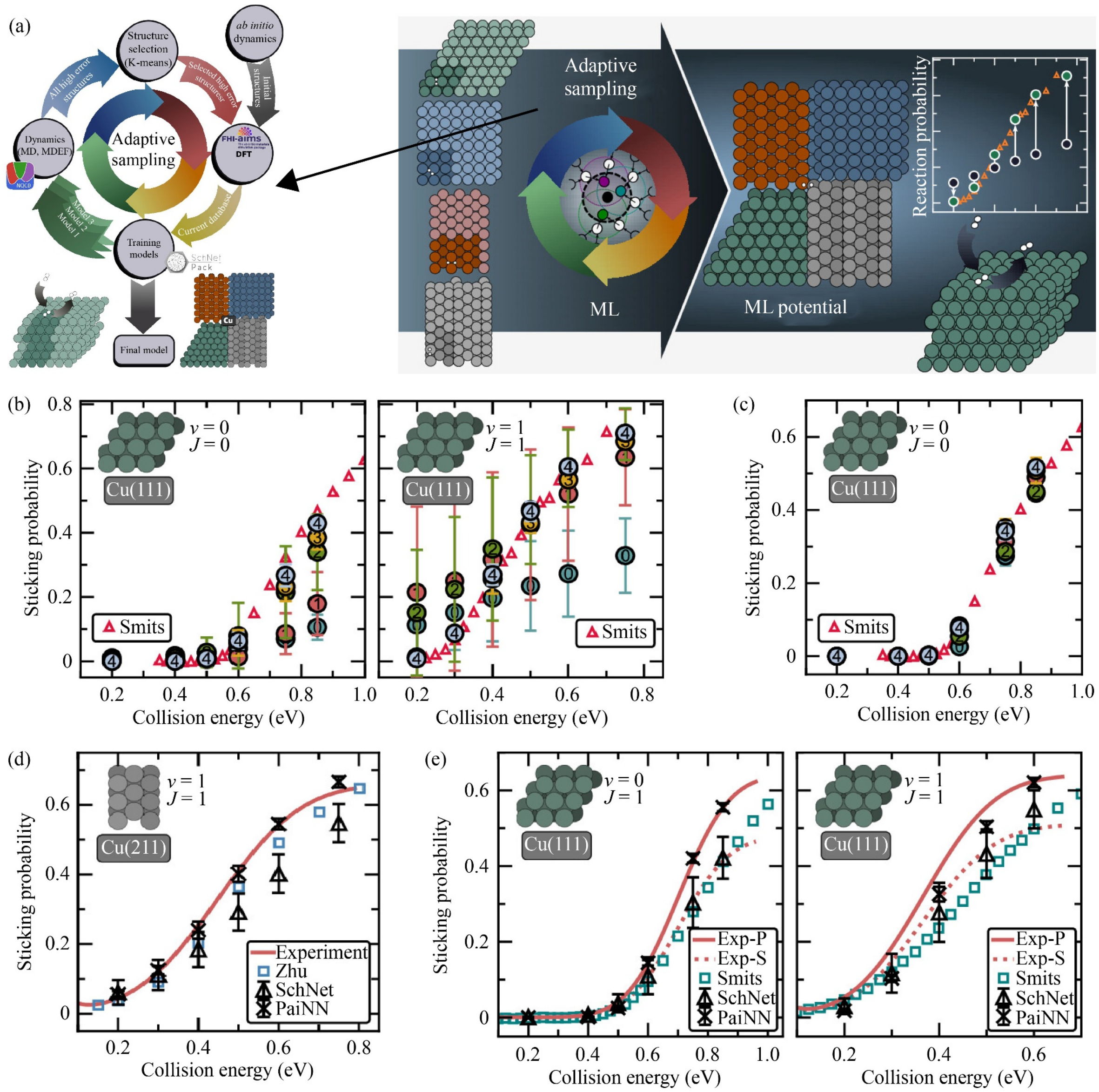

Fig. 13 (a) Workflow of the iterative adaptive-sampling scheme from an initial DFT set. (b, c) SchNet and PaiNN sticking probabilities for H_2/Cu(111) at 0 K (states as indicated) across adaptive-sampling iterations. (d) H_2/Cu(211) at 925 K ($v = 1$, $J = 1$): SchNet/PaiNN *vs*. EANN and experiment. (e) H_2/Cu(111) at 925 K for $v = 0$ and $v = 1$: SchNet/PaiNN *vs*. QCD-EAM-DCM (Smits & Somers) and experimental sticking functions. Reprinted with permission from Ref. [92], copyright 2023, American Chemical Society.

Collectively, these findings show that equivariant message-passing architectures, coupled with uncertainty-guided active sampling, can reliably predict dissociation and desorption probabilities with fewer DFT labels, offering a transferable paradigm for constructing reactive potentials across facets and temperatures.

Wille et al. [93] constructed an HDNN-PES (Behler-Parrinello) for H/D-graphene using ~7.6 × 10^4 PBE-D2 configurations with committee-based active learning, then ran ~10^6 scattering MD trajectories and benchmarked against angle-resolved energy-loss experiments. The PES captures a shallow physisorption well plus a chemisorption barrier/deep well and, across incident angles and isotopes, separates quasi-elastic scattering from the chemisorption-path energy-loss branch, outperforming REBO-EMFT. This provides an experimentally validated route where a single NNP-PES spans vdW adsorption and bond-forming chemisorption, linking well depth/barrier height to observables and supplying quantitative benchmarks for H_2 adsorption/dissociation/reversibility on storage surfaces.

For surface diffusion, Kataoka et al. [94] built a vibrating-surface Pd(111) model and trained a Behler-Parrinello-type NNP via self-learning hybrid Monte Carlo, combining quantum transition state theory (QTST) and ring-polymer molecular dynamics (RPMD) to compute D(T), 60–800 K. Results show non-Arrhenius, tunneling-dominated transport near 150–200 K and recrossing-induced lower RPMD diffusion coefficient than QTST at the higher temperature; including surface flexibility/multi-degree of freedom couplings reduces diffusion coefficient overestimation seen in frozen/reduced models. Under the same potential, surface and bulk diffusion are comparable up to 800 K with increasing subsurface branching, supporting NNP-based path-integral microkinetic modeling of adsorption/dissociation, diffusion, and recombination.

Focusing on the hydrogen-storage material magnesium, Morrison et al. [95] developed a Behler-Parrinello NNP for the Mg–H system and integrated a committee-based, uncertainty-driven active-learning strategy. Using a small but information-dense reference set, they achieved joint energy/force fitting of Mg–H interactions and, by evaluating paired energy- and force-errors in key configurational slices—H–H approach, surface/subsurface regions, and exit geometries—bolstered PES fidelity in both barrier regions and weak-interaction regimes (Figs. 14(a) and 14(b)). Building on this, they carried out NNP-MD on a thick MgH_2(110) slab at 800 K for 1 ns and, using an event-identification scheme based on H–H distance and layer index, constructed time series for each H_2 event, r(t) (H–H distance) and z(t) (depth coordinate/layer index). This enabled direct observation and statistics of a dehydrogenation sequence comprising subsurface molecular-hydrogen formation, residence (most events > 10 ps, with maxima > 60 ps), migration to the surface, and final desorption (Figs. 14(c–e)). Representative subsurface H_2 configurations captured by NNP-MD were then cross-checked by DFT geometry optimizations and 20 ps of DFT-MD at 800 K, and formation-energy comparisons (bulk-interior formation energies higher than near-surface subsurface) rationalized the thermodynamic driving force for facile formation and long residence (Figs. 14(f–i)). Methodologically, this articulates a closed-loop workflow based on energy/force-co-trained NNPs with uncertainty control, long-timescale MD with event identification, and DFT validation of key configurations, culminating in a coherent mechanistic synthesis.

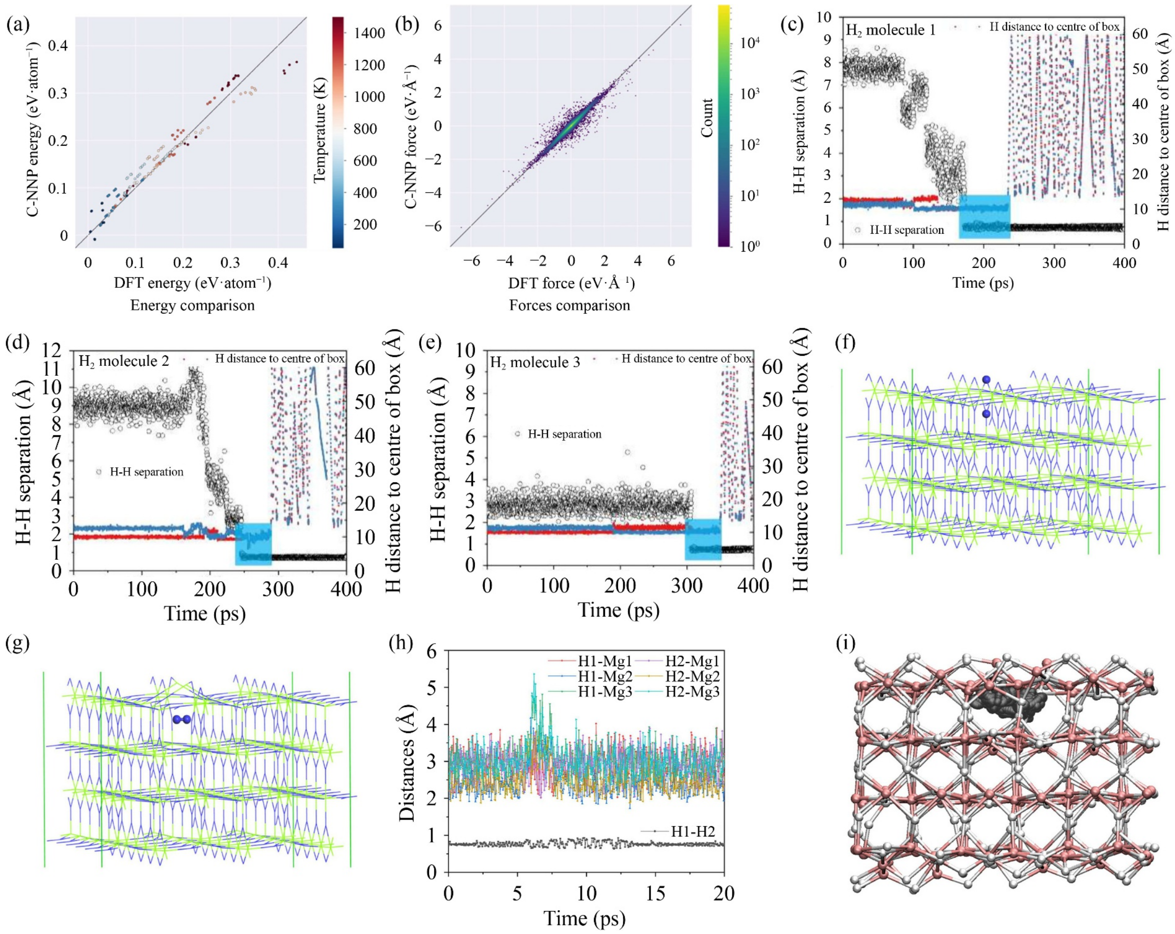

Fig. 14 (a, b) Parity plots comparing C-NNP with DFT for energies and forces. (c–e) Time evolution of interatomic distances for three selected H_2 molecules (M1–M3) on MgH_2(110); trapped states are highlighted (light-blue shading). Left axis: H–H distance (open circles); right axis: distance of each H from the box center (colored dots). (f, g) DFT-relaxed MgH_2(110) slabs (4-layer, 6 × 3 supercell): (f) perfect cell and (g) a cell containing a subsurface molecular H_2; atoms of interest are marked in blue. (h) Distances versus time between H1–H2 and between H1/H2 and neighboring Mg atoms (Mg1–Mg3). (i) Trajectories of H1 and H2 during DFT-MD. Green and blue sticks in (a) and (b), respectively. Mg and H atoms are represented in pink and white balls in (d), respectively. Reprinted with permission from Ref. [95], copyright 2024, American Chemical Society.

4.2.2 NNP-enabled bulk hydrogen transport: diffusion and migration

Ito et al. [96] addressed the limited accuracy of hydrogen diffusion predictions in random alloys by developing a ternary Ni–Mn–H machine-learning interatomic potential and coupling active learning with MD and nudged elastic band (NEB) calculations, yielding diffusion behavior in agreement with experiment. The observed non-monotonic dependence on Mn content is explained by the competition between lattice expansion, which lowers migration barriers, and Mn–H repulsion, which raises them. This study provides a transferable, methodological framework for MLP in ternary random alloys together with a mechanistic interpretation.

Wang and Huang [97] addressed the limited accuracy of hydrogen diffusion predictions in random alloys by developing a ternary Ni–Mn–H machine-learning interatomic potential and coupling active learning with MD and NEB calculations, yielding diffusion behavior in agreement with experiment. The observed non-monotonic dependence on Mn content is explained by the competition between lattice expansion, which lowers migration barriers, and Mn–H repulsion, which raises them. This study provides a transferable, methodological framework for MLP in ternary random alloys together with a mechanistic interpretation.

Liu et al. [98] address the long-standing difficulty of accurately modeling H_2–OMS (open metal sites) interactions—poorly captured by generic force fields—by training a DeepMD-based MLP for Al-soc-MOF-1d from AIMD-generated configurations and energies/forces (near-DFT accuracy; workflow in Fig. 15(a). This strategy targets the sub-class of MOFs with OMS where classical mixing-rule force fields fail, thereby enabling reliable, large-scale simulations of adsorption/diffusion that are otherwise prohibitive at the quantum level. With the trained MLP embedded in MD, the authors resolve adsorption structure and temperature-dependent dynamics at the pore-wall/OMS interface: H_2 preferentially localizes near Al-OMS with an equilibrium separation of ~2.7 Å, consistent with DFT and AIMD benchmarks, and progressively delocalizes with increasing temperature, reflecting modest binding, and enhanced mobility (radial distribution function (RDF)/trajectory evidence in Figs. 15(b) and 15(c)). The same MLP framework quantifies diffusion kinetics (Arrhenius analysis; Fig. 15(d)), linking OMS–H_2 specific interactions to reduced self-diffusivity relative to OMS-free MOFs.

4.3 Limitations and future needs

4.3.1 Limitations of local NNPs

Most existing NNPs approximate the PES based on atomic local environments within a finite cutoff radius. This ‘locality assumption’ enables efficient reproduction of local bonding and short-range interactions; however, it exhibits systematic deficiencies in scenarios involving long-range electrostatics and nonlocal charge transfer [99]. In the context of solid-state hydrogen storage and release, hydrogen adsorption, dissociation, and diffusion processes are strongly coupled with surface/interface characteristics, defects/grain boundaries, and phase transitions. These processes span multiple temporal and spatial scales, encompassing both the breaking and formation of chemical bonds at the electronic structure level and the cooperative motion of large numbers of atoms. These processes are frequently accompanied by inter-cell charge redistribution and variations in multiscale energy landscapes, which cannot be consistently and accurately described using purely local potentials. Consequently, recent studies have therefore focused on strategies to mitigate such limitations by incorporating global electronic effects while striving to maintain computational efficiency [89]. This direction is considered essential for improving the reliability of NNPs in solid-state hydrogen storage research.

4.3.2 Lack of generality across materials and conditions

In practice, in hydrogen storage and release studies, most NNPs are trained for a specific class of storage materials or under narrowly defined conditions (e.g., a single metal, alloy, or hydride crystal structure, specific temperature/pressure, or defect state). Such ‘specialized potentials’ typically yield accurate predictions within their training domains, but when applied across different materials, chemical compositions, or conditions (such as variations in temperature, hydrogen concentration, or surface/interface/defect structures), errors often increase significantly due to distribution shift. This lack of transferability limits their applicability for cross-system comparisons, property predictions, and new material screening in hydrogen storage research. Notably, some preliminary attempts have already been reported. For instance, in carbon–hydrogen systems, Ibragimova et al. [100] proposed a general MLP capable of handling a wide range of configurations from small molecules to solid-state materials, thereby demonstrating improved transferability across materials.

4.3.3 Training-set design and data sampling for NNPs

The reliability of NNPs for solid-state hydrogen storage hinges on training-set coverage across phases, surfaces/grain boundaries, defects, and rare transition states; small or biased sets trigger OOD errors. Active-learning workflows [101,102] can reduce this drift but still require explicit and calibrated uncertainty diagnostics and well-defined exploration policies. Long-range electrostatics and nonlocal charge transfer at metal–hydride interfaces challenge local descriptors, motivating charge-aware and equivariant models [103,104]; yet diversified

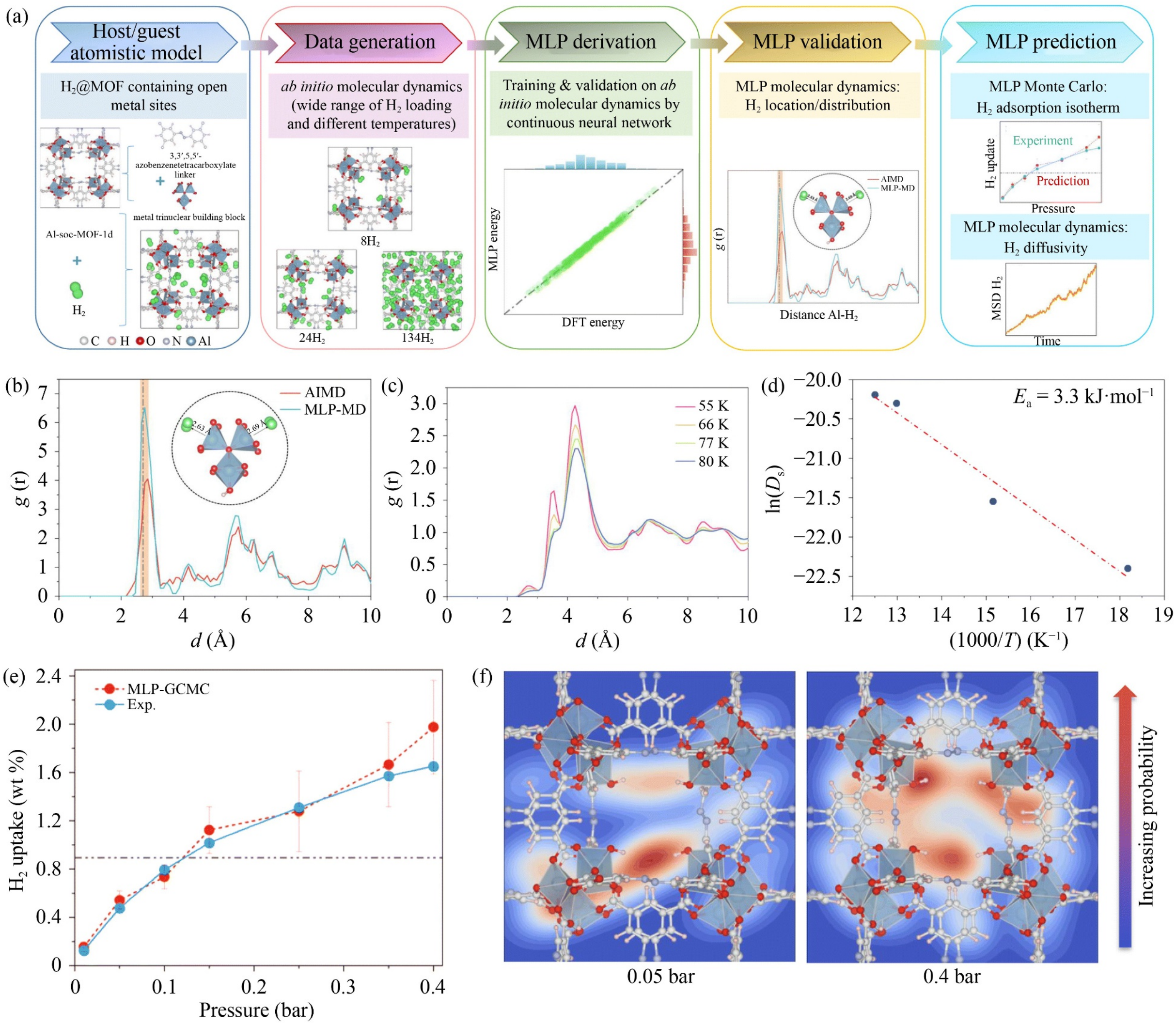

Fig. 15 (a) Workflow devised for the derivation and validation of a MLP for H_2@Al-soc-MOF-1d toward prediction. (b) RDFs calculated for the Al-OMS/H_2 pair by MLP-MD (light-blue) and AIMD (red) both performed at 10 K. The dashed line, located at approximately 2.7 Å, corresponds to the equilibrium Al-H_2 distance obtained in the DFT-geometry optimized structure (0 K). The inset delivers an illustration of these preferential interactions between H_2 and the Al-OMS site. (c) RDFs calculated for the Al-OMS/H_2 pair by MLP-MD simulations conducted at various temperatures (55, 66, 77, and 80 K, respectively). (d) Arrhenius plot of the self-diffusion for H_2 simulated by MLP-MD simulations. (e, f) MLP-GCMC prediction. (e) Simulated H_2 adsorption isotherms for Al-soc-MOF-1d (red symbols) vs. experimental volumetric measurements (blue symbols) at 77 K, ranging from 0.01 to 0.4 bar. (f) Simulated probability distribution of H_2 at 0.05 (left) and 0.4 bar (right), respectively. Reprinted with permission from Ref. [98], copyright 2024, Royal Society of Chemistry.

sampling and clear validity/applicability domains remain essential for defensible mechanistic claims.

5 Conclusions and outlook

Hydrogen energy is widely regarded as a crucial pillar of future clean energy systems, and the choice of hydrogen storage strategies directly determines the feasibility of its large-scale deployment. Among the various storage routes, solid-state hydrogen storage is widely considered promising due to its high volumetric density, intrinsic safety, and potential reversibility. Nevertheless, the development of solid-state hydrogen storage materials is highly complex, involving not only the thermodynamic stability and kinetic characteristics of hydrides but also the evolution of microstructures, cyclic stability, and compatibility with engineering applications. Conventional experimental studies and first-principles calculations have significantly advanced this field; however, their long research cycles, high costs, and limited scope hinder rapid iteration and large-scale screening. Against this backdrop, the introduction of ML has opened new opportunities by enabling efficient exploration across larger material spaces, thereby accelerating the design and mechanistic understanding of hydrogen storage materials in a data-driven paradigm.

This review summarizes recent progress in applying ML to solid-state hydrogen storage, with reference to insights derived from the Digital Hydrogen database. Current evidence indicates that ML has been successfully applied to predicting storage capacity, estimating absorption/desorption temperatures, and screening candidate materials, thereby supporting new material discovery and performance optimization. For instance, models based on SVM, RF, and GNN have achieved reasonable predictions of hydrogen storage performance using relatively small data sets. Moreover, strategies that integrate high-throughput computation with ML have shown the potential to accelerate large-scale screening. On the mechanistic side, NNPs have emerged as a promising approach, offering near-first-principles accuracy while greatly enhancing computational efficiency, and have been successfully applied to simulating local processes such as hydrogen diffusion and dissociation kinetics. Taken together, these advances suggest that ML is not only valuable for forward prediction and data mining but is also gradually penetrating deeper into mechanistic studies of hydrogen absorption and release.

Despite this progress, the application of ML in solid-state hydrogen storage remains at an early stage, far from fully supporting material discovery and engineering implementation. The current challenges are multifaceted. First, existing databases are limited in scale, with insufficient completeness and consistency to support high-accuracy models. Consequently, many studies still operate under 'small data' conditions, leading to limited generalizability, biased predictions, and a lack of systematic validation, while both extrapolation capability and interpretability remain underdeveloped. Furthermore, most efforts to date focus on performance prediction of known materials (i.e., forward design), whereas application-oriented inverse design strategies are still underdeveloped, limiting the ability to address engineering-driven requirements. At the mechanistic level, while NNPs have shown potential in simulating local processes such as diffusion and dissociation, their applicability remains narrow; comprehensive potentials capable of describing full hydrogen absorption-desorption cycles are still lacking. These issues highlight the considerable challenges facing the integration of ML and NNPs into solid-state hydrogen storage research. Looking ahead, as shown in Fig. 16, further improvements and expansions of ML applications in solid-state hydrogen storage are expected in the following aspects:

(1) Construction of open-access multimodal databases

Open-access multimodal databases are essential for advancing ML in solid-state hydrogen storage. Beyond conventional numerical parameters (e.g., capacity, temperature, pressure), future databases should integrate textual information from literature, numerical descriptors of thermodynamic and kinetic properties, and spectral or imaging data such as XRD/XPS curves, SEM (scanning electron microscope)/TEM images, and performance curves (PCT, DSC, isothermal kinetics). Standardizing and sharing such heterogeneous data will improve model accuracy, robustness, and reproducibility, while providing a foundation for developing multimodal learning frameworks that better capture structure-property-performance relationships.

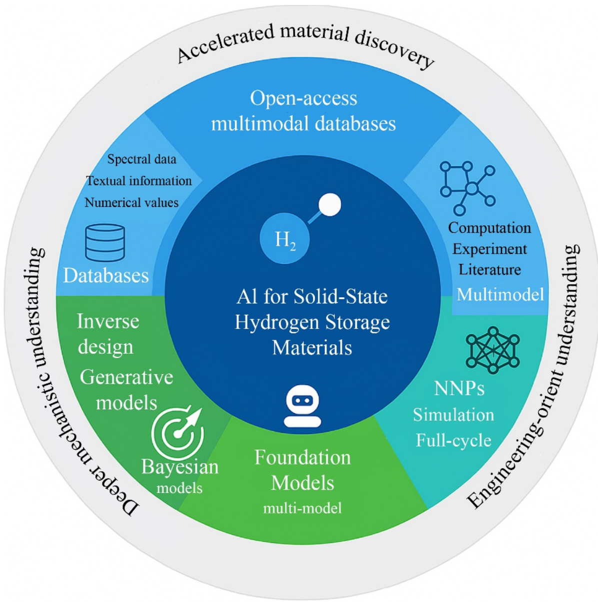

Fig. 16 Conceptual schematic of the outlook for solid-state hydrogen storage materials.

(2) Development of multimodal foundation models integrating experiments, computation, and data-driven methods

Solid-state hydrogen storage spans processes across electronic, atomic, and macroscopic scales, which no single approach can fully capture. Future progress requires multimodal foundation models capable of learning from diverse data sources, including textual knowledge from literature, numerical descriptors of thermodynamic and kinetic properties, and spectral or imaging data such as XRD/XPS curves and SEM/TEM images. By jointly leveraging these heterogeneous modalities and embedding them within a unified framework that integrates experimental evidence, first-principles calculations, and ML, such models can improve cross-scale prediction, enhance transferability, and accelerate practical materials discovery.

(3) Exploration of inverse design strategies driven by application requirements

Inverse design is a critical avenue for accelerating material discovery. By integrating generative models, evolutionary algorithms, and Bayesian optimization, ML has the potential to directly generate candidate material compositions tailored to specific application demands (e.g., high capacity, low-temperature reversibility, long cycle life). Such approaches would not only shorten research cycles but also facilitate the transition of solid-state hydrogen storage materials from laboratory research to engineering applications through explicit linkage between target properties and design constraints.

(4) Development of high-accuracy NNPs applicable to full hydrogen absorption-desorption cycles

The advancement of NNPs will provide more powerful tools for mechanistic studies of hydrogen storage. Future work should focus on overcoming the current limitations of NNPs in terms of material scope and process coverage, ultimately constructing generalized potentials capable of describing the complete hydrogen storage cycle. Moreover, optimization of training set selection and data sampling strategies will be essential to enhance the robustness and transferability of NNPs across diverse material systems. With progress in computational resources and methodological innovation, NNPs are expected to play an increasingly critical role in unraveling complex kinetic processes, supporting experimental interpretation, and guiding the rational design of novel materials.

In summary, solid-state hydrogen storage research is transitioning from traditional experience-driven paradigms toward data-driven methodologies. The integration of ML and NNPs is opening new avenues for both predictive modeling and mechanistic understanding, but their current capabilities remain limited and require further refinement. Future progress will hinge on the establishment of comprehensive databases, the construction of multi-scale and multimodal models, and the adoption of inverse design strategies tailored to practical demands. By systematically advancing these areas, data-driven approaches are expected to significantly accelerate material discovery and optimization, thereby reinforcing the role of solid-state hydrogen storage in the global clean energy transition.

Competing interests The authors declare that they have no competing interests.

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