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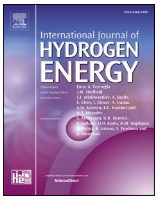

Digital Hydrogen-S: An open-access interactive Data platform for solid-state hydrogen storage materials

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ABSTRACT

Solid-state hydrogen storage is a promising technology due to its safety and high energy density. However, the absence of comprehensive and accessible data limits the accelerated development of high-performance materials. To address this challenge, we developed the *Digital Hydrogen-S* platform (http://digital-hydrogen.com/storage/), a large-scale, high-quality, open-access database dedicated to solid-state hydrogen storage materials. This platform integrates over 3,000 unique material entries and approximately 254,000 structured data records from more than 1,000 peer-reviewed publications. Its hierarchical data architecture ensures comprehensive coverage, standardization, and traceability of thermodynamic, kinetic, and compositional information. Equipped with interactive modules for data visualization, benchmarking, and user data entry, *Digital Hydrogen-S* enables multidimensional analysis and comparative exploration across diverse material systems. By facilitating data-driven materials design and performance optimization, this platform establishes a robust foundation for accelerating innovation in solid-state hydrogen storage research.

1. Introduction

In recent years, solid-state hydrogen storage has been widely regarded as one of the most promising hydrogen storage technologies due to its safety, high volumetric density, and broad operating temperature range [1,2]. However, the practical application of this technology is fundamentally limited by the performance of storage materials, which display diverse constraints across different classes, as exemplified by Mg-based hydrides that require high desorption temperatures, exhibit sluggish reaction kinetics, and possess limited reversibility [3–5].

Practical implementation of solid-state hydrogen storage technologies requires meeting a set of stringent, application-specific performance

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benchmarks [6–8]. For instance, Modi et al. [9] proposed that practical room-temperature hydrides should deliver a hydrogen capacity above 2 wt.%, achieve full hydrogen absorption and desorption within 3 min, and retain at least 70% of their capacity after 10,000 cycles. In addition, the DOE Technical Targets for Onboard Hydrogen Storage for Light-Duty Vehicles [10] specify that the system gravimetric capacity should reach 0.055 kg H_2/kg system by 2025, with an ultimate goal of 0.065 kg H_2/kg system. The acceptable hydrogen delivery temperature range is -40 °C to 85 °C, while the delivery pressure range is 5–12 bar. To meet these ambitious targets, extensive research efforts have focused on enhancing material performance through strategies such as catalysis [11], alloying [12], and nanosizing [13]. However, despite substantial progress, most reported materials still fail to satisfy all benchmark requirements simultaneously. Traditionally, material development has relied on trial-and-error experimentation, which is both time-consuming and inefficient in uncovering structure–property relationships [14]. As a result, this limitation has significantly constrained the pace of new material discovery.

With the rapid advancement of artificial intelligence, data-driven methods, particularly those based on machine learning, are emerging as powerful tools to accelerate material discovery. However, most existing studies in solid-state hydrogen storage still rely on datasets of relatively small scale, which inevitably restricts model generalizability and robustness. Although these approaches have achieved encouraging progress, several specific challenges remain, including insufficient data quantity, limited feature diversity, and skewed sample distributions. For instance, Kim et al. [15] collected hydrogen absorption Pressure-Composition-Temperature (PCT) data at 303 K for 33 different AB_2-type hydrogen storage alloys, yielding a raw dataset of only 506 points. To augment the training set, over 132,000 additional data points were generated via function fitting and the van't Hoff equation. Despite this expansion, the dataset remained significantly biased toward Ti-rich and Zr-rich systems, resulting in reduced prediction accuracy ($R^2 = 0.85377$) for balanced alloys such as $Ti_{0.515}Zr_{0.485}Mn_{1.2}Cr_{0.8}$. Lu et al. [16] employed ensemble learning to construct a structure–property relationship model for V–Ti–Cr–Fe alloys using 81 samples and 19 features encompassing composition and crystal structure. Although the model effectively predicted maximum hydrogen absorption capacity, the limited sample size and skewed distribution (with most values clustered between 2.0 and 3.5 wt.%) imposed constraints on model generalizability. Similarly, Zhou et al. [17] established a dataset of 234 C14 Laves-type high-entropy alloys for composition screening and capacity prediction, but the uneven distribution of key features such as Fe content and mean ionic charge compromised the model's accuracy ($R^2 \approx 0.806$). Dong et al. [18] used 183 and 113 samples with defined maximum hydrogen storage (Ab_max) and maximum hydrogen release (De_max) values, respectively, to model the hydrogen storage performance of Mg-based binary and ternary alloys. Despite achieving R^2 values of 0.947 (Ab_max) and 0.922 (De_max) on the test set, prediction errors in the validation set reached up to 22.57%. In addition, Dangwal et al. [19] used 420 literature-curated data points to train Gaussian Process Regression models predicting hydride formation enthalpy in Ti–Zr–Cr–Mn–Fe–Ni high-entropy alloys. Similarly, the MH-PCTpro framework was trained on 138 alloy compositions encompassing 237 PCT isotherms to predict full pressure–composition curves; although its leave-one-composition-out validation yielded approximately 80% success, the model's predictability was constrained by limited training diversity [20].

Since the inception of research in solid-state hydrogen storage, traditional experimental trial-and-error approaches have accumulated a substantial amount of performance data, thereby providing a strong foundation for large-scale data integration. However, these data remain fragmented across numerous publications, without a centralized, standardized, and openly accessible platform to fully exploit their value. This absence of a comprehensive, high-quality, and up-to-date database has become a critical bottleneck that restricts further progress in the field. Against this backdrop, it is necessary to evaluate the current status of existing solid-state hydrogen storage databases to identify their limitations and explore opportunities for building a next-generation data infrastructure.

Currently, the major databases for solid-state hydrogen storage materials include the Hydride Information Center (HydPARK) [21], Hydrogen Storage Materials Database [22], ML-HydPARK Dataset [23], Materials Project [24] and High Entropy Alloys Databases (TCHEA8) [25]. Among these, HydPARK is the most widely used, containing data on 2,722 hydrogen storage materials such as AB-, AB_2- and AB_5-type alloys. It integrates key hydrogen storage properties, including composition formula, hydrogen weight percent, heat of formation, hydrogenation temperature, and plateau pressure at room temperature. However, as the database has not been updated since 2002 and suffers from pervasive data incompleteness, its capability to support current research requirements is limited. The Hydrogen Storage Materials Database is essentially an extension of HydPARK. ML-HydPARK, derived from the original HydPARK database, has undergone extensive data cleaning and curation to remove duplicates and incomplete records. Nevertheless, similar to HydPARK, it also suffers from severe data lag. The Materials Project mainly provides physical properties such as composition and structural characteristics, without reporting key performance metrics like hydrogen capacity and desorption temperature, and all data are obtained from high-throughput computations rather than experiments. TCHEA7, developed by Thermo-Calc Software, is a thermodynamic and physical property database for high-entropy alloys (HEAs), covering 54 elements and providing calculated properties such as Gibbs free energy, specific volume, liquid viscosity, electrical resistivity, and thermal conductivity. However, access requires a paid license, which restricts its availability to the wider community. Overall, existing databases for solid-state hydrogen storage materials are generally limited by small data volume, low data quality, incomplete property coverage, and restricted accessibility, factors that have significantly hindered progress in related research.

Therefore, we assembled a dedicated team of 30 faculty members and graduate students from the Hydrogen Science and Engineering program at North China Electric Power University. Following a year of intensive collaborative effort, we successfully developed ***Digital Hydrogen-S*** (http://digital-hydrogen.com/storage/)—an open-access digital data platform focused on solid-state hydrogen storage materials. The platform currently hosts over 3,000 unique materials extracted from more than 1,000 peer-reviewed publications, totaling approximately 254,000 structured data entries. These data encompass a broad range of categories, including material composition, preparation methods, and key hydrogen absorption/desorption performance metrics. Furthermore, to address evolving research demands and foster data-driven innovation in hydrogen storage, the platform will be continuously maintained and regularly updated.

2. Database design and construction

The ***Digital Hydrogen-S*** (http://digital-hydrogen.com/storage/) platform currently contains over 3,000 unique material entries sourced from more than 1,000 peer-reviewed publications, comprising over 254,000 structured data entries spanning a broad range of material systems and performance categories. These encompass critical properties such as enthalpy, entropy, and plateau pressure, together with experimental PCT and kinetic curves. The dataset also contains metadata detailing material composition and modification methods.

The launch of the *Digital Hydrogen-S* database effectively addresses the growing research demand in the field of solid-state hydrogen storage. As shown in Fig. 1(a), the temporal distribution of journal publications related to solid-state hydrogen storage demonstrates a steady upward trend from 2000 to 2024. After 2014, the annual number of publications rose significantly, with rapid growth observed after 2020. From 2021 to 2023, publication counts reached consecutive new highs,

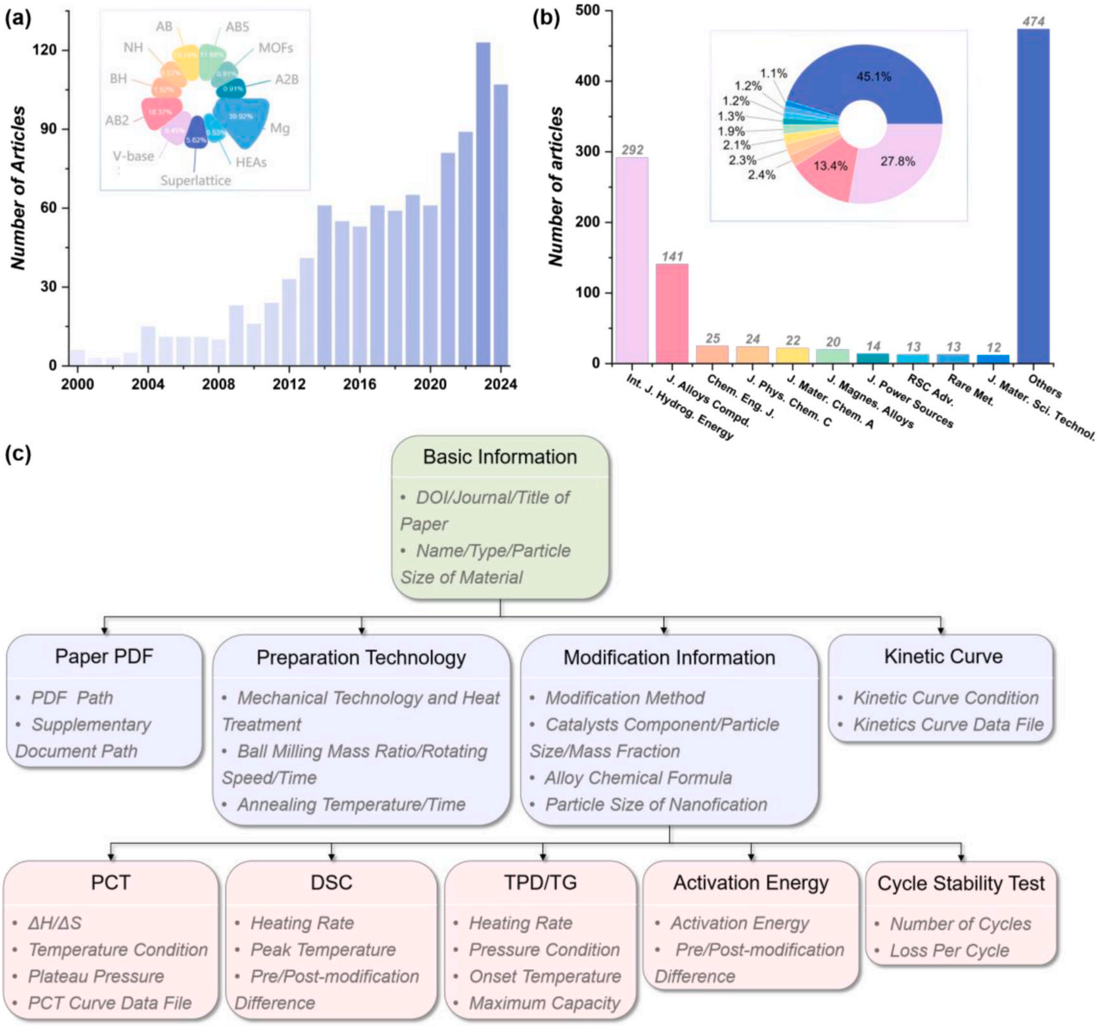


Fig. 1. (a) Annual distribution of platform-indexed literature (2000–2024), with an embedded rose chart depicting the proportional distribution of hydrogen storage material types. (b) Literature distribution across journals, presented as a bar chart with an inset pie chart employing the same color scheme; the legend is omitted for clarity. (c) Structural framework diagram of the database. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

with a year-on-year growth rate of 38% in 2023. Notably, although the number of entries recorded for 2024 shows a 13% decline compared to 2023, this figure may be underestimated due to delays in literature indexing. This overall trend reflects the growing global emphasis on hydrogen energy and the increasing research interest in solid-state hydrogen storage technologies.

Complementing the temporal publication trends, an analysis of the material composition within the database provides further insight into the research emphasis across different solid-state hydrogen storage systems. Fig. 1(a) also presents the composition of the database, which encompasses eleven material categories, including AB, AB_2, AB_5, Mg-based hydrides, V-based solid solutions, superlattice (SL), borohydrides (BH), nitrogen-based hydrides (NH), A_2B-type compounds, high-entropy alloys (HEAs), and metal–organic frameworks (MOFs), totaling 3,296 materials. Mg-based materials constitute the largest share (39.92%), followed by AB_2-type (18.37%) and AB_5-type (11.68%) alloys, highlighting their sustained prominence in hydrogen storage research. In contrast, newer classes of materials such as HEAs (0.53%) account for smaller proportions, indicating that despite growing interest, these systems remain relatively underexplored. Additionally, materials that have been extensively studied for decades, such as BH (1.29%), NH (0.57%), and MOFs (0.91%), also show relatively small proportions, mainly due to the current underrepresentation of related data in the database, which will be addressed through ongoing expansion and updates.

To ensure scientific rigor and data reliability, the majority of entries in the database are curated from internationally recognized journals indexed by authoritative repositories such as the Web of Science Core Collection (SCIE) and Scopus. After retrieving the literature, we further conducted manual screening to retain only highly relevant publications. Although the current number of source articles is approximately 1,000, this rigorous process has resulted in more than 254,000 structured and high-quality data entries, reflecting the exceptional depth and precision of the database. As shown in Fig. 1(b), the distribution of source articles across different journals reveals that the top ten journals by article count are *International Journal of Hydrogen Energy* (*Int. J. Hydrog. Energy*), *Journal of Alloys and Compounds* (*J. Alloys Compd.*), *Chemical Engineering Journal* (*Chem. Eng. J.*), *Journal of Physical Chemistry C* (*J. Phys. Chem. C*), *Journal of Materials Chemistry A* (*J. Mater. Chem. A*), *Journal of Magnesium and Alloys* (*J. Magnes. Alloys*), *Journal of Power Sources* (*J. Power Sources*), *RSC Advances* (*RSC Adv.*), *Rare Metals* (*Rare Met.*), and *Journal of Materials Science and Technology* (*J. Mater. Sci. Technol.*). Collectively, these journals contribute 54.9% of the total literature included in the database. In particular, *Int. J. Hydrog. Energy* accounts for the largest share with 292 articles (27.8%), followed by *J. Alloys Compd.* with 141 articles (13.4%). Additionally, each dataset entry in the database is associated with a unique Digital Object Identifier (DOI), enabling users to directly access the original source through the platform's integrated interface. This traceability mechanism significantly enhances the transparency and credibility of the database.

Notably, it is worth emphasizing that this database employs a more systematic information architecture, featuring a hierarchical structure that progressively organizes and expands material data to comprehensively encompass various performance parameters of solid-state hydrogen storage materials (see Fig. 1(c)). As illustrated in the figure, the database is structured into three distinct layers. The first layer provides a basic description of the source literature. The second layer contains detailed material information and enriched bibliographic metadata. The third layer focuses on recording a wide range of hydrogen absorption and desorption performance parameters. This layered design guarantees a rigorous and organized documentation process for each material entry.

Building upon this hierarchical and systematic information architecture, the database not only ensures structured organization but also incorporates critical experimental data to enhance the depth and usability of each material entry. Specifically, it integrates key information such as pressure–composition–temperature (PCT) curves, kinetic curves, synthesis parameters, and hydrogen absorption/desorption performance, adopting a multimodal data structure that enables comprehensive characterization from multiple dimensions. To validate the comprehensiveness and reliability of the performance parameters recorded in this database, a multidimensional comparison was conducted with HydPARK, a widely used and authoritative database in the field of solid-state hydrogen storage. As shown in Table 1, the results indicate that this database provides more detailed and standardized thermodynamic and kinetic parameters, reflecting a higher level of data specificity and professionalism. Furthermore, each material entry contains both hydrogen absorption and desorption data, significantly enhancing the completeness and applicability of the dataset. In addition to manually curated databases, emerging AI-based workflows such as the Descriptive Interpretation of Visual Expression (DIVE) [26] have been developed to extract data from scientific figures. However, their current applications in solid-state hydrogen storage remain limited in data volume and accessibility, whereas the *Digital Hydrogen-S* platform provides openly available, manually validated data with broader coverage and higher reliability.

Moreover, to facilitate user engagement and enhance accessibility, an introduction video (http://digital-hydrogen.com/storage/operation-en.html) has been prepared to demonstrate the main features, data architecture, and functionalities of the *Digital Hydrogen-S* platform. Provided as an attachment, the video presents a step-by-step guide for navigating the interface, searching for materials, and performing comparative analyses.

Table 1
Comparison of critical parameters of materials included in this database with HydPARK.

	Material Parameters	HydPARK	*Digital Hydrogen-S*
Material Composition	Chemical Composition Formula	✓	✓
	Catalysts Component/Particle Size (nm)/Mass Fraction (wt.%)	×	✓
	Particle Size (nm) of Nanofriction	×	✓
Preparation Process	Ball-to-powder Ratio/Ball-milling Rotating Speed/Time	×	✓
	Annealing Temperature/Time	×	✓
Thermodynamic Properties	PCT ΔH ($kJ \cdot mol^{-1}$)	✓	✓
	PCT ΔS ($J \cdot mol^{-1} \cdot K^{-1}$)	×	✓
	PCT Temperature (°C)	×	✓
	Plateau Pressure(bar)	✓	✓
Kinetic Properties	DSC Heating Rate($^{\circ}C \cdot min^{-1}$)	×	✓
	Peak Temperature (°C)	×	✓
	Activation Energy ($kJ \cdot mol^{-1}$)	×	✓
	Cycle Performance Cycles	×	✓
	Loss Per Cycle(wt.%)	×	✓
Others	Maximum Capacity(wt.%)	✓	✓
	Onset/Initial Temperature (°C)	×	✓

3. Web interface and usage

3.1. Database design overview

To facilitate systematic storage, access, and management of solid-state hydrogen storage data, the *Digital Hydrogen-S* platform utilizes a modular, layered architecture that distinctly separates frontend user interaction from backend data processing. A screenshot of the platform's homepage is shown in Fig. 2(a), highlighting the main functional modules and user interface layout. As illustrated in Fig. 2(b), the system architecture comprises five logical layers: the access layer, frontend user interface layer, and interaction layer forming the frontend, alongside the backend service layer (implemented with the Flask framework) and the underlying MySQL database.

The frontend is developed using standard web technologies, including HyperText Markup Language (HTML), Cascading Style Sheets (CSS), and JavaScript (JS). HTML defines the page structure, CSS controls the visual appearance, and JS manages interactive functions and communication with the backend. Libraries such as ECharts (a JavaScript-based visualization library) and jQuery (a lightweight JavaScript framework) enable dynamic data visualization through interactive charts and tables, improving overall user experience. User requests are exchanged with the backend through Application Programming Interfaces (APIs) using Hypertext Transfer Protocol (HTTP) methods, where POST is used for data submission and GET for data retrieval, forming the core of frontend–backend interaction.

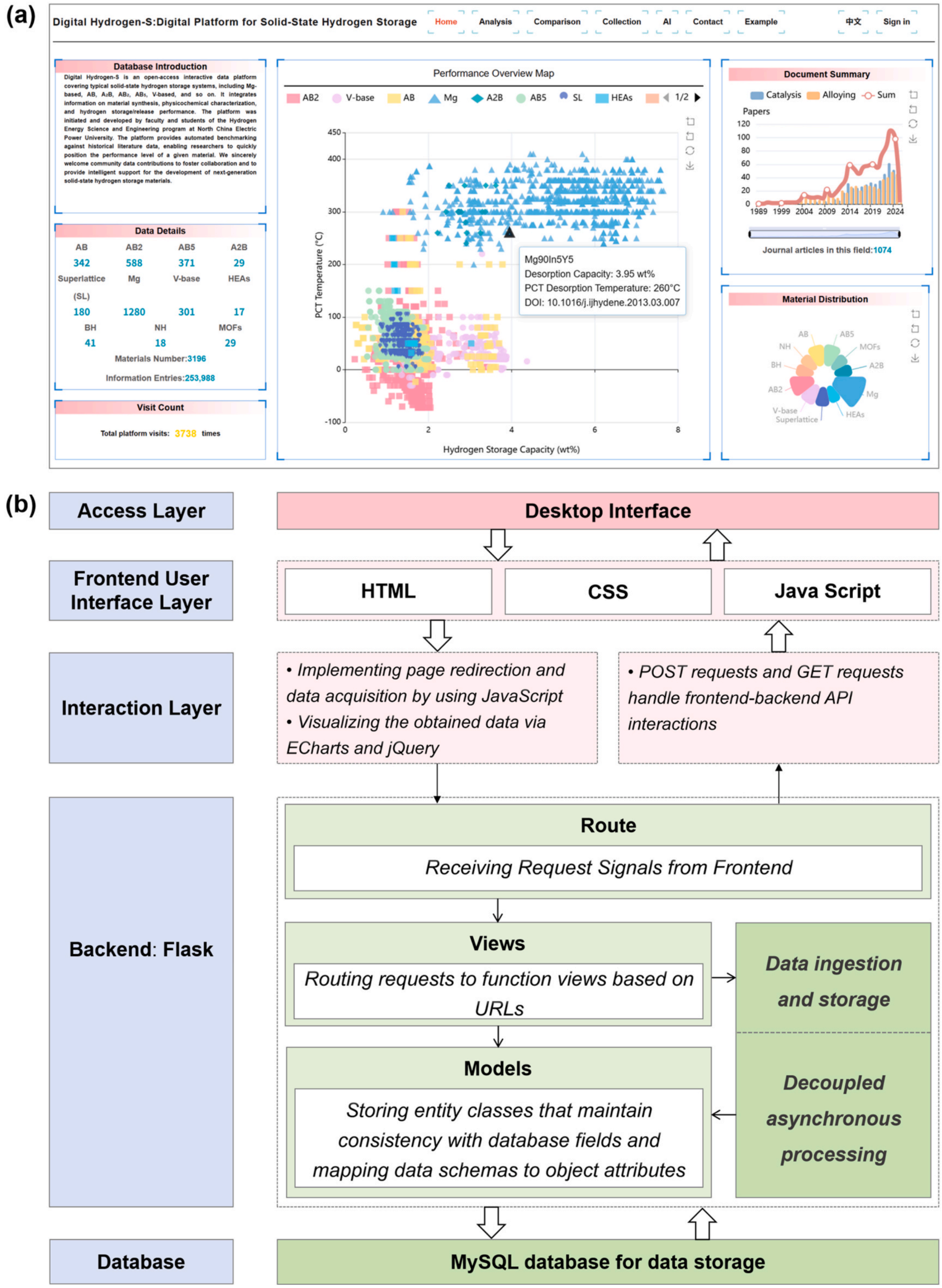
The backend adopts a Model–View–Controller (MVC) design pattern implemented in Flask (a lightweight Python web framework). Incoming requests are routed to view functions responsible for executing business logic and interacting with data models defined through SQLAlchemy Object Relational Mapping (ORM). These models correspond to normalized relational tables in the MySQL (My Structured Query Language) database, which stores comprehensive data including material compositions, synthesis techniques, modification strategies, and hydrogen storage performance metrics. Rigorous foreign key constraints and indexing mechanisms are employed to ensure data integrity and efficient query performance. Furthermore, asynchronous (non-blocking) processing modules handle computationally intensive tasks such as batch data validation and file parsing, thereby improving backend responsiveness and scalability.

This layered architecture provides maintainability, extensibility, and secure real-time access to an increasingly complex dataset of solid-state hydrogen storage materials. Fig. 2(a) depicts the overall frontend-backend framework and illustrates the data flow across the system layers.

3.2. Data entry

To uphold the principles of openness, collaboration, and sharing, the *Digital Hydrogen-S* platform implements a data entry function. By registering on the website, users can access this function and contribute relevant data to the platform. The specific operational procedure is detailed in Fig. 3.

As shown in Fig. 3, although the data entry process involves multiple steps, its design remains clear and systematic. First, a DOI-based duplication check streamlines the user experience by preventing redundant data submissions and reducing database redundancy. Second, the user interface is concise and logically organized to align with the typical experimental workflow in hydrogen storage materials research,



Database Introduction

Digital Hydrogen-S is an open-access interactive data platform covering typical solid-state hydrogen storage systems, including Mg-based, AB, A_2B, AB_2, AB_5, V-based, and so on. It integrates information on material synthesis, physicochemical characterization, and hydrogen storage/release performance. The platform was initiated and developed by faculty and students of the Hydrogen Energy Science and Engineering program at North China Electric Power University. The platform provides automated benchmarking against historical literature data, enabling researchers to quickly position the performance level of a given material. We sincerely welcome community data contributions to foster collaboration and to provide intelligent support for the development of next-generation solid-state hydrogen storage materials.

Data Details

AB	AB2	AB5	A2B
342	588	371	29
Superlattice (SL)	Mg	V-base	HEAs
180	1280	301	17
BH	NH	MOFs	
41	18	29	

Materials Number:3196

Information Entries:253,988

Visit Count

Total platform visits: 3738 times

Mg90In5Y5
Desorption Capacity: 3.95 wt%
PCT Desorption Temperature: 260°C
DOI: 10.1016/j.ijhydene.2013.03.007

Journal articles in this field:1074

Fig. 2. (a) Homepage interface of *Digital Hydrogen-S* platform. (b) Architectural diagram of *Digital Hydrogen-S* web platform's frontend-backend framework.

enabling users to efficiently extract and input data within a single session. To ensure data reliability and academic integrity, the platform incorporates a backend review mechanism in which all entries undergo expert verification by professors and graduate students specializing in hydrogen energy science and engineering. The review process follows clearly defined review criteria: (1) all submitted data must originate from publicly available and peer-reviewed literature; (2) the data format must comply with the standardized input templates of the platform; (3) reported values must be accurate, logically consistent, and clearly traceable. During the review process, each data entry is cross-checked against the original publication to confirm the correctness of numerical values, experimental conditions, and units. Only entries that fully meet these criteria are approved and officially recorded in the database. Submissions containing correctable issues are returned to the user through the personal revision system for modification and resubmission, while invalid or unverifiable entries are removed by the backend.

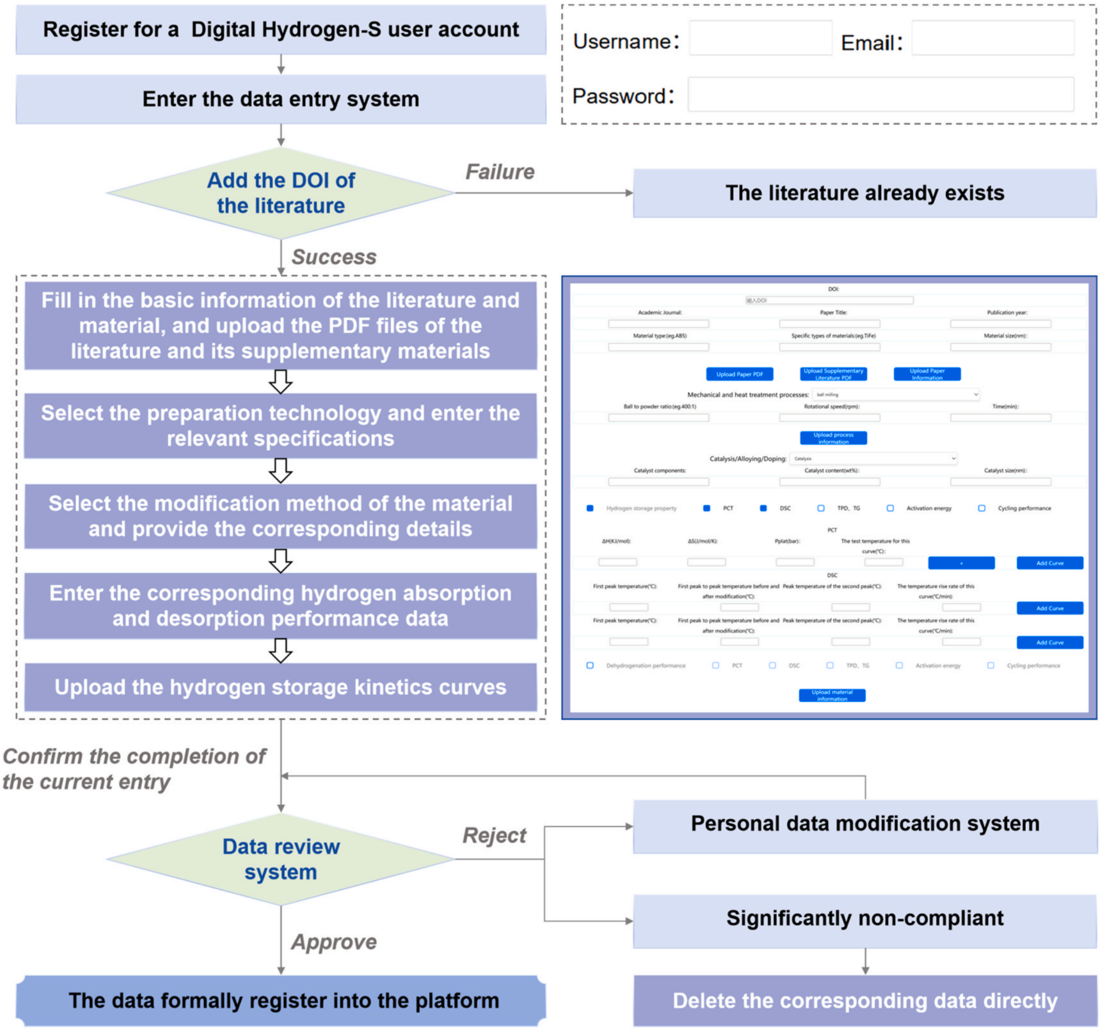


Fig. 3. Data entry workflow architecture of the *Digital Hydrogen-S* platform.

Furthermore, users can also provide feedback without submitting data through the Contact section, where the contact email of the project leader and a Quick Response (QR) code for the discussion group are available for addressing any platform-related issues, including those concerning the data. Such feedback channels help ensure continuous improvement of the platform's functionality and data quality. To maintain the timeliness of the database, the platform follows a monthly release cycle to publish newly approved entries and ensure continuous updates for users.

Data security and user privacy are also core priorities in the platform's design and implementation. A comprehensive, multi-layered security framework has been established, covering aspects such as user authentication, permission control, password encryption, and input validation. For instance, the platform employs a server-side session-based authentication system, integrates Cross-Site Request Forgery (CSRF) protection and password complexity policies, and implements account lockout mechanisms to defend against common cyber threats. Additionally, role-based access controls restrict users to managing only their own data records, while administrators are granted full access for platform oversight. This security framework not only ensures comprehensive protection of user data, but also effectively balances usability with operational safety.

3.3. Data Visualization Analysis

To facilitate data-driven exploration and intuitive performance comparisons of solid-state hydrogen storage materials, the platform features an interactive Data Visualization Analysis module. This tool enables users to dynamically filter, map, and analyze key material parameters within a visualized environment, thereby uncovering patterns and correlations that may not be evident in tabular formats.

By selecting desired performance variables for the X- and Y-axes in the left-side configuration panel, users can generate corresponding scatter plots in the display area (as shown in Fig. 4(a) and (b)). Hovering over a data point reveals detailed information such as DOI, material name, and values of the selected parameters, allowing personalized exploration of material-level data.

In Fig. 4(a), the dehydrogenation peak temperature is assigned to the X-axis and activation energy to the Y-axis—both critical kinetic parameters in hydrogen storage research. Many studies use the Kissinger method to estimate activation energies based on peak temperatures. As illustrated, most materials with reported values for these parameters are Mg-based materials. The activation energy values exhibit a wide range, from approximately 50 to 304.45 kJ·mol^{-1}, while the dehydrogenation peak temperatures mostly fall between roughly 80 °C and 450 °C.

Notably, the scatter plot supports multidimensional interactive mapping to enhance analytical capabilities. As shown in Fig. 4(b), plateau pressure is indicated by a color gradient—darker shades represent higher values. Meanwhile, hydrogen storage capacity controls the size of each point, with larger points corresponding to higher capacities. This visualization enables quick identification of materials with extreme values. For example, the material $Nd_5Mg_{85}Al_{10}$ exhibits the highest

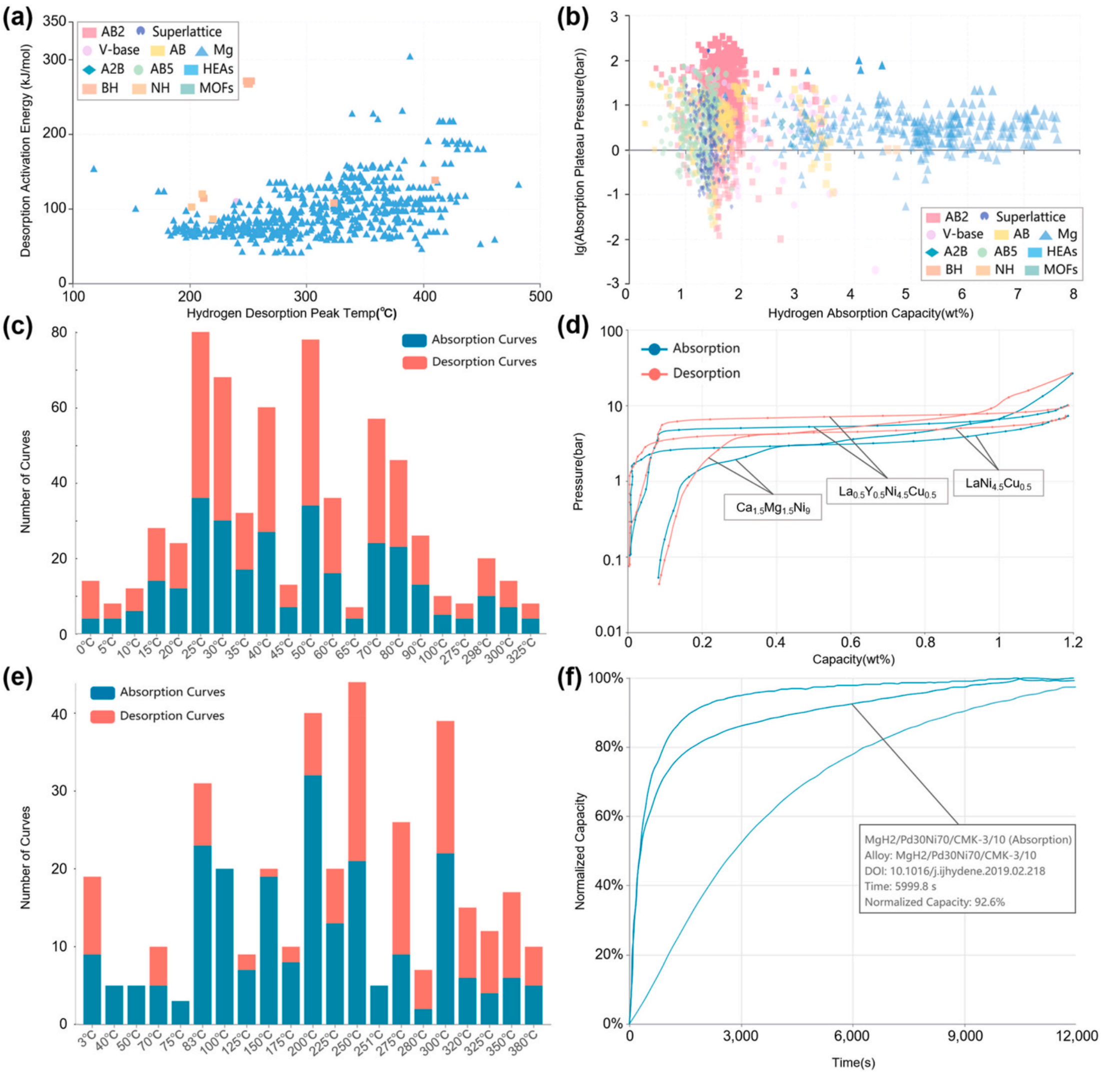


Fig. 4. (a) Scatter plot of dehydrogenation peak temperature versus activation energy. (b) Scatter plot of hydrogen storage capacity versus plateau pressure. (c) Distribution of PCT curves under different temperature control conditions. (d) PCT curves of various hydrogen storage materials measured at 45 °C for comparative analysis. (e) Distribution of kinetic curves under different temperature control conditions. (f) Hydrogenation kinetic curves of various hydrogen storage materials measured at 70 °C for comparative analysis.

hydrogen capacity of 7.58 wt.% alongside a relatively low plateau pressure of just 5.465 bar.

Although the performance of this material appears promising in these two metrics, it is important to note that scatter plots inherently provide limited information and omit key influencing factors such as temperature. Since both hydrogen capacity and plateau pressure depend on temperature, evaluating performance requires careful consideration of testing conditions.

To enable further thermodynamic comparisons across different materials, the platform includes a PCT Curve Comparison section. Fig. 4(c) presents the distribution of PCT curves recorded at temperature conditions for which more than five valid curves were available after data screening. A more detailed statistical distribution is provided in the Supporting Information. Each bar in Fig. 4(c), as an integral part of the comparison module, corresponds to a specific temperature; by selecting a temperature, users can generate comparison plots of multiple materials measured at that temperature in the lower display area (see Fig. 4 (d)). To improve visualization clarity, hydrogen absorption and desorption curves are differentiated by color. These plots not only display equilibrium pressure and capacity at a fixed temperature but also illustrate the full pressure–composition behavior throughout the absorption and desorption process.

Moreover, to support kinetic performance comparisons, the platform provides a Kinetic Curve Comparison section. Fig. 4(e) shows the distribution of kinetic curves on the platform under different temperature control conditions, based on selected temperature points where more than five curves are available. A more detailed statistical distribution is provided in the Supporting Information. Selecting a given temperature displays the kinetic curves of multiple materials measured at that temperature (Fig. 4(f)). To reduce interference from absolute capacity differences, the vertical axis (hydrogen absorption/desorption capacity) is normalized for all materials. As shown in the figure, hovering the cursor over any point on a curve reveals detailed information such as the corresponding material name and the DOI of the source document.

3.4. Data Benchmarking

To support systematic evaluation and screening of solid-state hydrogen storage materials, the platform incorporates a Data Benchmarking module that enables direct comparison between user-defined target values and the existing dataset. In experimental research, benchmarking against established performance thresholds, such as dehydrogenation temperature or hydrogen capacity, is critical for identifying promising candidates and refining design strategies. By providing a flexible and interactive comparison interface, this module facilitates evidence-based material assessment and enhances decision-making in hydrogen storage studies.

In the Data Benchmarking module, users can define target performance values, including hydrogen desorption peak temperature and hydrogen desorption capacity, via the configuration panel. Upon submission, the platform renders a scatter plot that incorporates the input as a benchmark point within the context of the full dataset. This functionality enables quantitative comparison between user-defined objectives and experimentally reported material data. To facilitate dissemination and reuse of analytical results, the Data Benchmarking module supports the direct export of all visual outputs (see Fig. 5).

As illustrated in Fig. 5, the red star denotes the newly input data point, positioned at 300 °C and 6 wt.%. This point falls within the dense distribution of Mg-based materials, which typically exhibit initial dehydrogenation temperature of 150∼350 °C and capacities of 5.5∼7.5 wt.%. The benchmark value, therefore, lies within the established property envelope of this material class. By embedding target points into a comprehensive comparative landscape, the platform supports evidence-based evaluation of material feasibility and guides future material design strategies.

By enabling seamless integration of benchmark analysis visuals into academic workflows, the platform enhances research efficiency and improves the transparency of material performance comparisons.

3.5. *AI chat*

The AI Chat module is positioned as an intelligent question–answering and analysis system powered by a large language model (LLM, GPT-4o). In contrast to simple database retrieval, it can automatically transform natural language questions into database queries and, when necessary, generate visual charts or textual reports. Such capabilities not only significantly enhance the interactivity of the *Digital Hydrogen-S* platform but also strengthen its role in research support, making it particularly well-suited for rapid problem solving and personalized analysis in solid-state hydrogen storage studies.

To clarify how these capabilities are realized, Fig. 6(a) presents the workflow of AI Chat, which outlines the decision-making logic and internal data flow. Upon receiving a natural language query, the system first determines whether access to the database is required. When database interaction is necessary, the LLM sequentially performs text-to-SQL conversion, query sanitization, and execution, followed by parsing the results into structured data. Within this process, three key decision points are emphasized: (i) whether a database query is needed, (ii) whether the query result is empty, and (iii) which output mode is selected by the user. To ensure accurate interpretation and reliable processing of queries, the workflow incorporates four distinct interactions with the LLM, namely generating general knowledge responses, performing text-to-SQL conversion, selecting appropriate chart types automatically, and producing data analysis reports. Depending on the decision flow, AI Chat can provide either interactive data visualizations generated through automated chart selection and Plotly rendering, or textual analytical reports, thereby supporting flexible modes of scientific insight delivery.

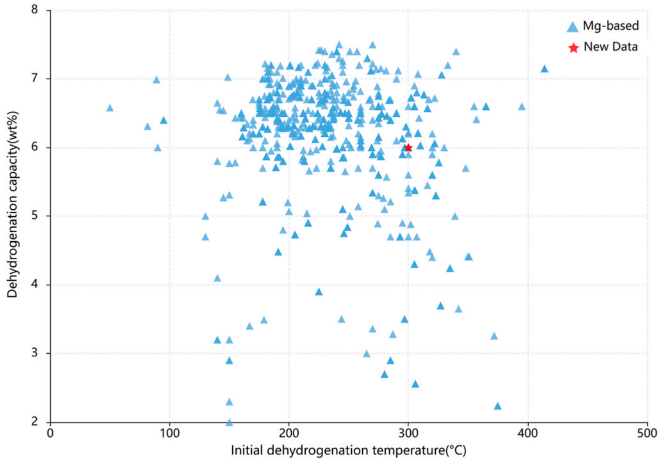


Fig. 5. Comparison of new and existing data in the scatter plot of initial dehydrogenation temperature versus dehydrogenation capacity.

Building on this workflow, a practical example of this functionality is depicted in Fig. 6(b), where the query “display the absorption temperatures after adding different catalysts and the corresponding values when MgH_2 is used as the modified material” was submitted. The system autonomously parsed the analytical intent, generated the SQL query, and retrieved relevant data for visualization. In the resulting output, a bar chart was produced that compares the initial desorption temperatures of 25 different catalysts. Notably, NiO/C (nickel oxide supported on carbon) [27] exhibited the lowest absorption temperature, underscoring its superior thermodynamic performance in this catalytic system. Moreover, the platform allows users to access the underlying raw data tables associated with each visualization, thereby ensuring transparency of analysis and enabling further data validation and in-depth exploration.

4. Statistical characteristic analysis based on data

To demonstrate the scientific utility and application potential of the *Digital Hydrogen-S* platform, this section presents a series of data-driven analyses based on the integrated database. Specifically, through multi-dimensional visualization and comparative exploration of key parameters, the platform enables researchers to uncover latent patterns, evaluate material trade-offs, and guide rational material design. In particular, the following analyses focus on representative visualizations that highlight performance distributions across material classes, thereby offering insights into inherent relationships and identifying promising candidates for future hydrogen storage development.

Fig. 7(a) illustrates the distribution of various hydrogen storage materials with respect to their PCT operating temperature and hydrogen capacity. Solid-state hydrogen storage materials exhibit distinct trade-offs between capacity and temperature performance across material categories. Magnesium-based materials demonstrate the highest hydrogen storage capacity, reaching up to 7 wt.% but typically require operating temperatures exceeding 200 °C, thereby constraining their suitability for low-temperature environments and increasing associated energy consumption. Vanadium-based solid solutions exhibit moderate storage capacities, ranging from 2 to 4 wt.%, with comparatively lower dehydrogenation temperatures of 0∼150 °C, making them suitable for medium-to low-temperature applications with reduced operational energy demands. AB-series alloys (including AB-, A_2B-, AB_2-, AB_5-type and superlattices) generally possess lower hydrogen capacities, ranging from 0 to 3 wt.%, but cover a wide temperature range, with a notable concentration in the 0∼100 °C region, reflecting their widespread use as traditional hydrogen storage alloys. Borohydrides (BH) and amide–hydride (NH) compounds exhibit relatively low capacities but operate at elevated temperatures, whereas emerging materials such as high-entropy alloys (HEAs) display broad temperature coverage and potential for optimization through compositional engineering.

Fig. 7(b) presents a scatter plot of hydrogen desorption enthalpy (ΔH, $kJ{\cdot}mol^{-1}$) versus entropy (ΔS, $J{\cdot}mol^{-1}{\cdot}K^{-1}$) for the same material categories, highlighting their thermodynamic characteristics. AB-, AB_2-, AB_5-type alloys and superlattices form a dense cluster in the region of moderate exothermic enthalpy, ranging from -10 to -80 $kJ{\cdot}mol^{-1}$, and entropy values between -50 and -150 $J{\cdot}mol^{-1}{\cdot}K^{-1}$, reflecting stable thermodynamic behavior suitable for moderate-temperature operation.

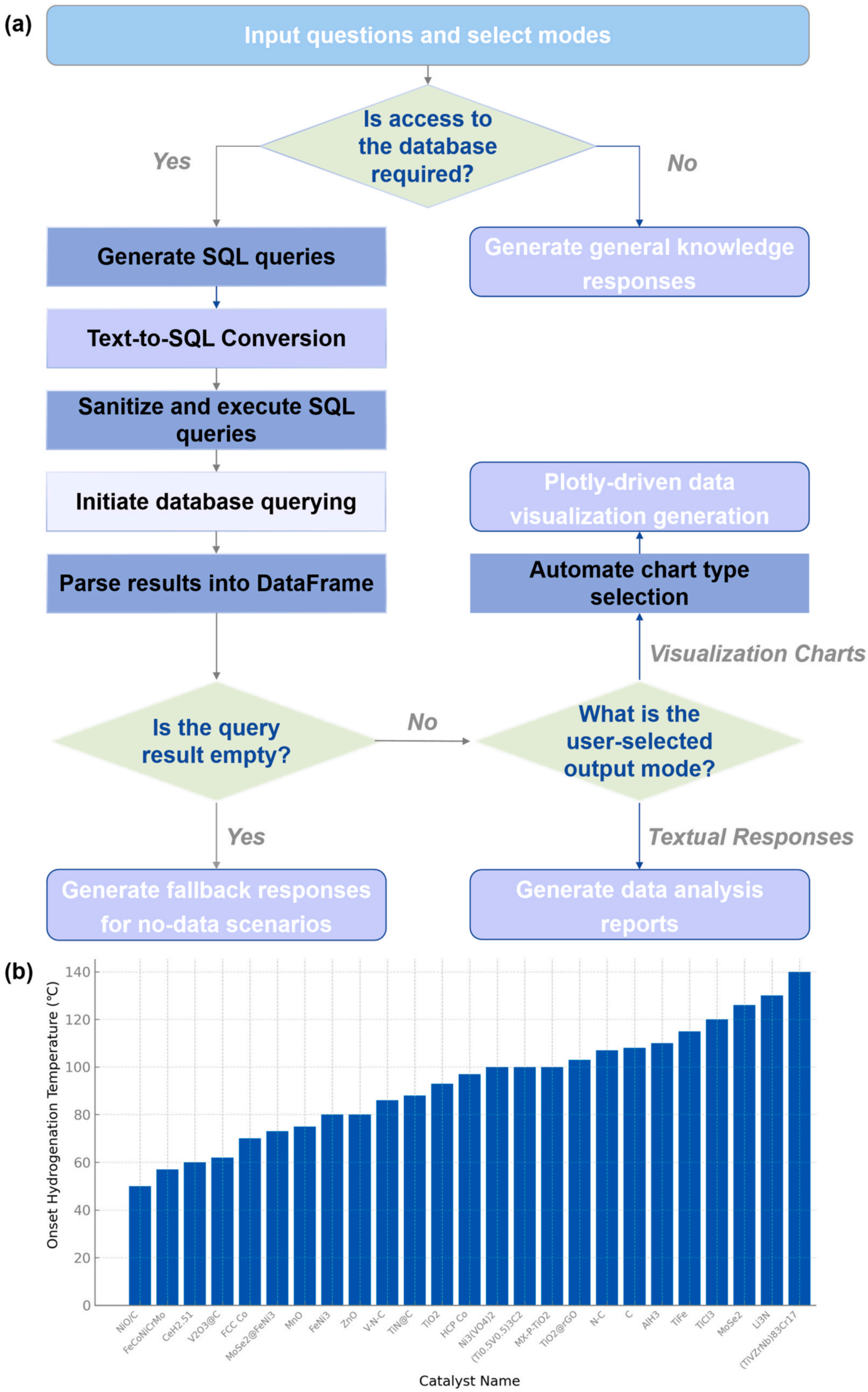


Fig. 6. (a) The workflow of the AI Chat based on large language models. (b) The catalysts added and the corresponding onset hydrogenation temperatures when MgH_2 was used as the modified material.

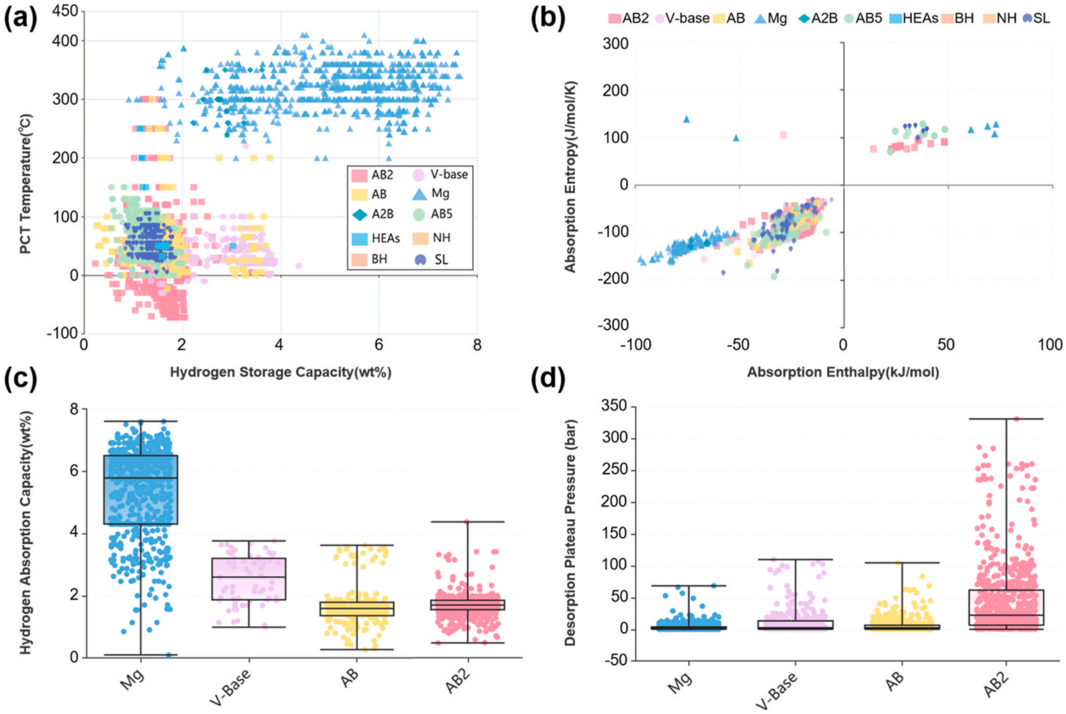


Fig. 7. (a)The distribution of various hydrogen storage materials in terms of their operating temperature and hydrogen capacity. (b)Scatter plot of hydrogen desorption enthalpy (ΔH, kJ·mol^{-1}) versus entropy (ΔS, J·mol^{-1}·K^{-1}) for various solid-state hydrogen storage materials. (c) Boxplot of hydrogen absorption capacity for different hydrogen storage material classes. (d) Boxplot of desorption plateau pressure for different hydrogen storage material classes.

Among these, AB_5-type alloys generally exhibit slightly higher entropy than AB_2-type materials, likely due to their inherently higher configurational disorder and hydrogen mobility. In contrast, Mg-based and A_2B-type alloys display broader thermodynamic ranges. While Mg_2Ni-based alloys predominantly fall near $\Delta H \approx -70$ kJ·mol^{-1}, several Mg-based hydrides extend into regions with substantially higher or even positive enthalpy and entropy, suggesting metastable states or compositional variations. V-based solid solutions and HEAs exhibit scattered distributions without clear clustering, indicating either intrinsic compositional complexity or limited dataset coverage. Outliers with positive ΔH or unusually high ΔS may result from experimental uncertainties or data quality variability. Conventional intermetallic exhibit well-established thermodynamic properties, whereas Mg-based and complex multicomponent alloys offer a wider design space that requires further optimization.

Building upon these thermodynamic and temperature–capacity insights, Fig. 7(c)–(d) provide a statistical overview of hydrogen absorption capacity and desorption plateau pressure across major material categories, enabling comparative evaluation of their storage potential and operational requirements. Mg-based hydrides show the highest median capacity, approximately 5.8 wt.%, with low desorption pressures (median approximately 1 bar), attractive for high-density storage under near-atmospheric conditions, though kinetic limitations remain. V-based solid solutions present moderate capacities, with a median of approximately 2.6 wt.%, and broader pressure variability, while AB-type alloys exhibit lower capacities, with a median of approximately 1.6 wt.% and predominantly low pressures with occasional high-pressure outliers, indicating niche applicability. A_2B alloys, despite a small dataset, display narrow capacity and pressure ranges. AB_2-type alloys combine modest median capacities of approximately 1.7 wt.% with the widest pressure span, ranging from near-atmospheric conditions to above 300 bar, highlighting adaptability and heterogeneity. AB_5-type alloys and other emerging materials provide complementary strengths, particularly in capacity–pressure combinations. These analyses reveal that Mg-based materials dominate in capacity performance, AB_2-type alloys excel in pressure tunability, and AB-series intermetallics offer predictable behavior. These insights underscore the value of combining thermodynamic, kinetic, and operational data for rational material selection and provide guidance for future material design and hydrogen storage optimization.

In summary, the statistical analysis based on the integrated *Digital Hydrogen-S* database reveals notable trends and patterns across various material categories. The temporal distribution of research activity demonstrates both the well-established nature of traditional hydrogen storage systems and the rapid rise of emerging material classes. Comparisons of thermodynamic and kinetic properties further highlight the intrinsic trade-offs and design challenges associated with different alloy systems. By offering a comprehensive, standardized, and up-to-date dataset, the platform not only deepens the understanding of material performance but also facilitates data-driven discovery and optimization in the field of solid-state hydrogen storage. This analysis thus lays a solid foundation for guiding future research efforts and accelerating the development of advanced hydrogen storage materials.

5. Conclusion

In summary, the *Digital Hydrogen-S* (http://digital-hydrogen.com/storage/) platform offers a comprehensive, standardized, and up-to-date data infrastructure for solid-state hydrogen storage materials. It effectively addresses critical challenges such as data fragmentation, limited accessibility, and inconsistent data reporting by integrating a high-quality, large-scale dataset with advanced visualization and benchmarking tools. The platform's hierarchical data structure and interactive interface allow detailed performance comparisons, thermodynamic and kinetic analyses, and informed material design. Moving forward, we plan to continuously expand material categories, integrate operando characterization data, and enhance data standardization, all aimed at further increasing the platform's utility for the research community. Overall, *Digital Hydrogen-S* serves as a valuable open-access resource, facilitating data-driven discovery and accelerating the development of high-performance hydrogen storage materials.

CRediT authorship contribution statement

Wenfeng Fu: Writing – original draft, Methodology, Funding acquisition, Formal analysis, Conceptualization. **YanXin Li:** Writing – original draft, Project administration, Methodology, Data curation, Conceptualization. **Zhaoyan Dong:** Software, Resources, Data curation. **Jun Li:** Project administration, Methodology, Conceptualization. **Rui Liu:** Software, Data curation. **Yang Yang:** Software, Data curation. **Jiongyang Li:** Software, Data curation. **Leping Zhang:** Software, Data curation. **Chongbo Wang:** Investigation, Data curation. **Tongao Yao:** Investigation, Data curation. **Jianghao Cai:** Investigation, Data curation. **Zhuoran Xu:** Investigation, Data curation. **Haoqi Tian:** Investigation, Data curation. **Yuan Gao:** Investigation, Data curation. **Zhuohang Fu:** Investigation, Data curation. **Jiangbao Lin:** Investigation, Data curation. **Haokun Huang:** Investigation, Data curation. **Jinwen Xu:** Investigation, Data curation. **Yuhan Du:** Investigation, Data curation. **Xianjie Yang:** Investigation, Data curation. **Jiahang Li:** Investigation, Data curation. **Haobo Wang:** Investigation, Data curation. **Qi Zhao:** Investigation, Data curation. **Jingjuan Guo:** Investigation, Data curation. **Chunyan Huang:** Investigation, Data curation. **Yiluo Ding:** Investigation, Data curation. **Jinhao Xu:** Investigation, Data curation. **Xiangyu Song:** Investigation, Data curation. **Junyi Wo:** Investigation, Data curation. **Boyang Liu:** Investigation, Data curation. **Xinyu Huo:** Investigation, Data curation. **Yujie Yan:** Investigation, Data curation. **Lei Liao:** Investigation, Data curation. **Kang Ma:** Investigation, Data curation. **Tangxuan Gao:** Investigation, Data curation. **Junwei Zhao:** Investigation, Data curation. **Mengni Zhang:** Investigation, Data curation. **Ze Liu:** Investigation, Data curation. **Rui Chang:** Investigation, Data curation. **Jie Shu:** Investigation, Data curation. **Junming Huang:** Investigation, Data curation. **Junyu Lin:** Investigation, Data curation. **Yankun Wang:** Investigation, Data curation. **Meiyi Wang:** Investigation, Data curation. **Chengkai Yuan:** Investigation, Data curation. **Guanjiu Wu:** Investigation, Data curation. **Xuqiang Shao:** Software. **Zhengyang Gao:** Writing – review & editing, Supervision. **Yuan Li:** Investigation, Data curation. **Jia Hu:** Investigation, Data curation. **Yakun Zhu:** Investigation, Funding acquisition, Data curation. **Weijie Yang:** Writing – review & editing, Supervision, Resources, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.ijhydene.2026.153434.

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