

Role of compositionally complex and high entropy alloys for hydrogen storage: A bibliometric and mechanistic assessment

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ABSTRACT

Compositionally complex and high entropy alloys have emerged as promising candidates for hydrogen storage in the transition towards sustainable energy systems. This study provides a comprehensive bibliometric and systematic review of HEA-based hydrogen storage, analysing 214 publications from the Scopus database (2010–2024). Using VOSviewer, the analysis identifies key research trends, influential authors, and collaborative networks while pinpointing research gaps. Results highlight the dominance of BCC and Laves phase HEAs due to their superior hydrogen storage capacities, structural stability, and tunable thermodynamic properties. Mechanistic insights reveal that high configurational entropy, severe lattice distortions, and sluggish diffusion significantly impact hydrogen absorption/desorption kinetics. Computational modeling and machine learning are identified as crucial for accelerating alloy design and optimization. Challenges remain, including slow kinetics, limited cycling stability, and activation requirements. Overcoming these challenges necessitates interdisciplinary research, focusing on optimizing storage capacity and kinetics, investigating microstructural influences, and expanding datasets for improved machine learning predictions. This study integrates bibliometric and mechanistic insights, providing a valuable resource for researchers and practitioners. By addressing these challenges and fostering global collaboration, HEAs can pave the way for the widespread adoption of hydrogen energy and contribute significantly to sustainable energy innovations.

1. Introduction

Renewable energies are crucial for a sustainable future. These energy sources such as wind, solar and hydrogen emit little to no greenhouse gases during application unlike fossil fuels. Renewable energies are essential in addressing climate changes and ensuring a reduction in the usage of carbon emitting energy sources. Additionally, renewable energies enhance energy security by diversifying our energy mix and reducing reliance on fossil fuels, thereby stabilizing energy prices and promoting economic growth. They aid in creating employment and scientific innovation in the clean technology sectors, driving economic development while preserving natural resources and ecosystems. Embracing renewable energies is a necessity for combating global warming [1,2]. These energy sources provide efficient pathway towards a cleaner, healthier, and more sustainable planet for future generations.

Hydrogen energy represents a promising frontier for sustainable and renewable energy solutions. This is due to its abundant source, clean,

carbon emission free and high gravimetric energy density [3–7]. Despite the merits associated with hydrogen as energy carrier, the safe, efficient, and storage challenge is one of the main barriers to realizing a hydrogen-based economy [3,7,8]. Among the various strategies, solid-state metal hydrides for hydrogen storage using has shown promise due to its inherent safety, reversibility, and volumetric efficiency [7,9]. Thus, the search for novel hydride materials that combine high storage capacity, fast kinetics, and cyclic durability is critical.

Hydrogen can be stored by means on physical based storage or by material-based storage as shown in Fig. 1. Hydrogen storage by means of absorption in metal hydrides is a storage technology with potential for various applications. Storage via metal hydrides offers high volumetric energy densities and better safety due to hydrogen being able to be chemically bound at relatively low temperatures [10]. Metal hydrides present a promising technology for various applications due to its high volumetric energy density and improved safety, as hydrogen can be chemically bound at lower temperatures [10]. While pure metals like magnesium can store significant amounts of hydrogen (up to 7.65 wt%

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Acronyms/abbreviations

HEA	High Entropy Alloy
RHEA	Refractory High Entropy Alloy
CCA	Complex Concentrated Alloys
CALPHAD	CALCulation of PHase Diagram
BCC	Body Centered Cubic
FCC	Face Centered Cubic
HCP	Hexagonal Close Packed
SDG	Sustainable Development Goal
VEC	Valence Electron Concentration
AM	Arc Melting
BM	Ball Milling

HEBM	High Energy Ball Milling
LENS	Laser Engineered Net Shaping
MA	Mechanical Alloying
RM	Reactive Milling
wt %	Weight Percentage
H/M	Hydrogen to Metal Ratio
ML	Machine Learning
SVM	Support vector machines
NN	Neural network
RF	Random Forest
GPR	Gradient Process Regression
DFT	Density Functional Theory
VASP	Vienna Ab Initio Simulation Program

at 250–450 °C), they exhibit poor kinetics and cyclability [11]. Efforts to enhance the performance of Mg through alloying can improve these aspects but often result in a trade-off with hydrogen storage capacity. Alloys such as LiBH₄ (18.5 %), Mg (BH₄)₂ (14.8 %) and NaBH₄ (10.6 wt %) show greater hydrogen storage capabilities than pure metals, yet they face challenges like thermodynamic instability and low recyclability [12].

Compositionally complex alloys (CCAs) and high entropy alloys (HEAs) offer a disruptive pathway for next-generation hydrogen storage materials. The compositionally complex alloys are defined by the multi-principal elemental compositions, which exhibit unique features such as high configurational entropy, severe lattice distortions, cocktail effects and sluggish diffusion [14–18]. These characteristics contribute synergistically to enhanced hydrogen absorption, phase stability, and tunable thermodynamic properties [19–25]. In particular, BCC-structured CCAs/HEAs present abundant interstitial sites which are either tetrahedral or octahedral, favouring hydrogen uptake [5,6,26,27]. Although, there are encouraging advances, the fundamental mechanisms governing hydrogen behaviour in these complex systems are barely understood, especially at the microstructural and atomic

scales [4,5,21,23,28–35]. Hence has become a subject area of intense research and investigation.

Current research lacks a systematic mapping of trends, collaboration networks, and predictive frameworks for CCA/HEA hydrogen storage. Although many studies report specific HEA compositions [29,36–50] and performance metrics [4,6,7,20–23,28,31–33,35,51–60], there is a limited effort to distil global research patterns or to integrate computational approaches such as first principle density functional theory (DFT), traditional and physic-based machine learning approaches for rational alloy design [3,8,61]. The absence of a holistic perspective hampers the rational design and rapid discovery of HEA-based hydrides optimized for practical applications. Additionally, challenges such as slow kinetics, surface degradation, and cyclic instability remain largely unresolved. For instance, Ti₂₅V₃₀Cr₅Mn₄₀ achieved a storage capacity of 3.99 wt% at 80 °C [62], whereas TiZrFeMnCrV, designed via CALPHAD, showed fast kinetics and excellent cyclic stability at room temperature with hydrogen stabilization at 1.76 wt% after 50 cycles [63]. Although, there have been recent reviews on hydrogen storage properties of published HEAs, manufacturing route, thermodynamics HEAs along with the microstructural characteristics of alloy systems [64–67].

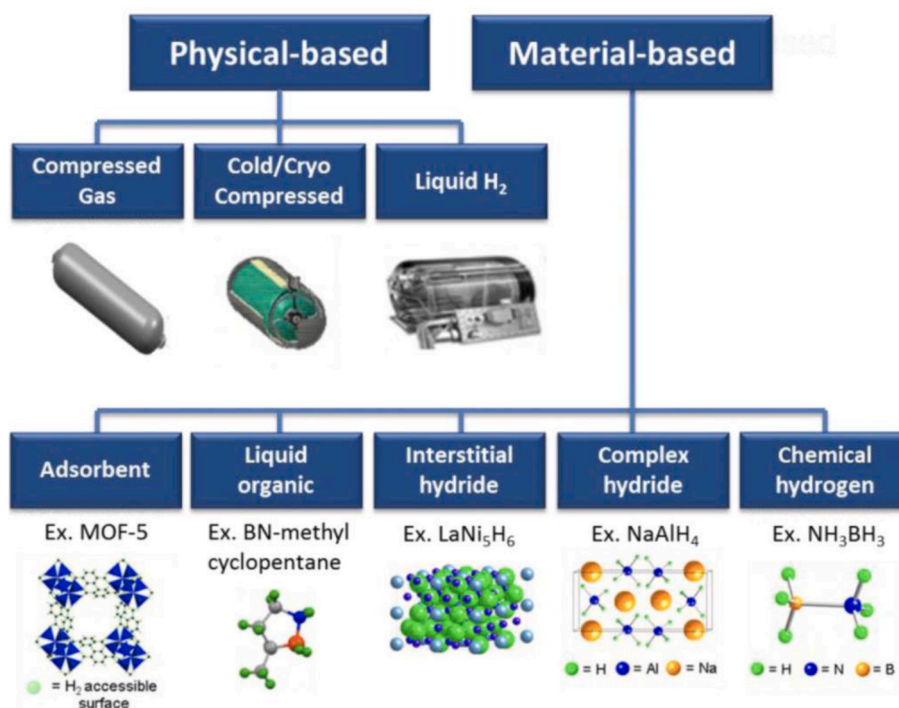


Fig. 1. Hydrogen storage methods based on physical and material-based media [13].

These review paper look into the There is however a scarcity of bibliometric work devoted to investigating, assessing and visualising CCA-s/HEAs hydrogen storage literature from a global view coupled with recent mechanistic insights and advancement.

This review aims to address existing gaps in the field of HEA/CCA hydrogen storage through a twofold approach. First, a comprehensive bibliometric analysis is conducted to assess research evolution, map out collaboration networks among institutions and countries, identify influential contributors, and uncover emerging research trends from 2010 to 2024. Using VOSviewer software, keyword co-occurrence is evaluated, high-impact publications highlighted, and knowledge gaps to guide future research directions outlined. Second, a detailed mechanistic review examines the core effects of CCAs/HEAs including high-entropy stabilization, severe lattice distortions, sluggish diffusion, and cocktail effects and their influence on hydrogen absorption, desorption, and stability. Particular attention is given to the role of microstructure, phase transformations, and defect engineering. By integrating bibliometric insights with mechanistic understanding, this work provides a strategic roadmap for advancing CCA/HEA-based metallic hydrides for hydrogen storage. The potential of emerging tools such as machine learning-assisted alloy discovery, high-throughput computational screening, and advanced characterization techniques to accelerate innovation and commercial deployment of HEA/CCA metal hydrides within the hydrogen energy sector are further emphasized.

2. Methodology

By utilising the results of academic research within a specific scientific discipline, bibliometric analysis generates networks of citations between authors, journals, and countries, analyses of co-authorship among authors, and co-occurrence of keywords.

2.1. Data mining strategy

The schematic flowchart used to complete the bibliometric and systematic review of hydrogen storage using HEA is given in Fig. 2. The Scopus database was used to retrieve article publications for hydrogen storage dating from 2010 to May 2024. Even though Web of science provides similar coverage, Scopus was chosen because it offers a vast and increased coverage of peer reviewed literature citations and abstracts. To retrieve relevant Titles, abstracts along with keywords

regarding to hydrogen storage using HEA, certain keywords were used in the Scopus database. The query string used was TITLE-ABS-KEY (hydrogen AND storage AND high AND entropy AND alloys) AND PUBYEAR >2009 AND PUBYEAR <2025 AND (LIMIT-TO (LANGUAGE, "English")) AND (EXCLUDE (DOCTYPE, "re")). The query string resulted in 214 articles which were extracted from the Scopus database.

2.2. Text cleaning

Through scrutinising the title abstracts and keywords of the 214 articles that were retrieved, irrelevant ones were identified and eliminated. Out of the 214 articles extracted, ~171 were irrelevant to hydrogen storage by mean of HEA. Open Refine, an open - source software was used to for text cleaning before processing in VOSviewer to glean insights.

2.3. Bibliometric analysis

A bibliometric review is a systematic analysis of the academic literature within a specific field or topic area, focusing on quantitative measures and patterns derived from bibliographic data. It involves identifying and analysing various bibliometric indicators such as journal impact factors, authorship patterns, publication trends, and citation counts. By synthesizing this information, a bibliometric review provides insights into the development, impact, and structure of research within a particular discipline or research area. It helps researchers and scholars understand the scholarly landscape, track the influence of key papers or authors, and identify emerging trends or gaps in the literature [68].

A bibliometric review provides valuable quantitative insights into academic output, revealing publication trends, citation patterns, and knowledge dissemination within a field. It enables researchers and institutions to assess impact, identify influential authors, seminal papers, and leading journals, and make informed decisions about future research directions. Additionally, bibliometric analyses help evaluate research productivity and the effectiveness of funding policies or academic programs. By systematically analysing bibliographic data, bibliometric reviews foster collaboration, map intellectual development, and strategically guide the advancement of knowledge across disciplines [69].

The publication growth trends were analyzed alongside comprehensive bibliometric assessments after data cleaning. Network maps

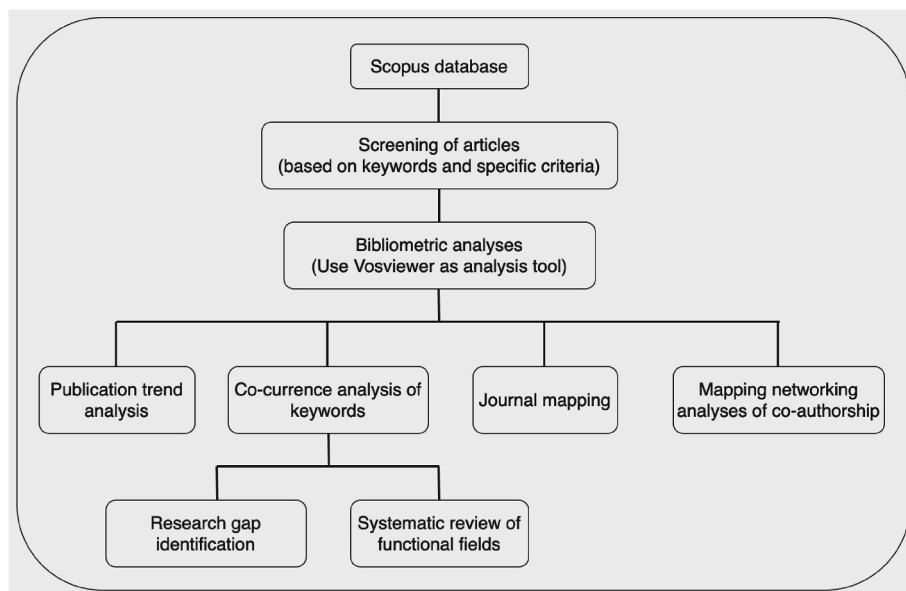


Fig. 2. Flow chart for bibliometric analyses.

were generated to show keyword co-occurrence, article and journal co-citations, and international co-authorship patterns. These analyses identified key research themes, collaboration networks, citation patterns, and influential publication outlets. All mapping was conducted using VOSviewer 1.6.17, a distance-based and open-source visualization tool where proximity indicates stronger relationships between nodes representing journals, authors, or countries. Larger nodes denote higher influence based on metrics such as document count and citation frequency. Clustering by colour indicates closely related research activities, while density visualizations highlight areas with greater publication volume or citation impact within CCA/HEA hydrogen storage research.

3. Results

3.1. Trend of publications of hydrogen storage using HEA from 2010 to May 2024

The yearly publication based on HEA as hydrogen storage materials is summarized in Fig. 3. This information was gathered from the Scopus database, whereby an inconsistent in publications can be observed from the year 2010 (first HEA alloy used for hydrogen storage) to year 2018, from the year 2019 there has been a gradual increase in hydrogen storage by means of HEA publications. This increase coincides with the adoption for the December 2015 Paris agreement and sustainable development goals that seek to reduce global emission by half in the year 2030. Research in HEAs as hydrogen storage material is expected to increase as HEA alloys show promising hydrogen storage properties and can aid in the reduction of emissions.

3.2. Preferred journals for publishing

It is important to identify journals that are prominent and subject matter specific. The identification processes are done to help aid researchers and funders to recognize up to date sources, map out recurring information and help in the formations of new ideas and efforts of their own. The reputation of the journal has proven to enhance the chances of citation. The article network map of the top 20 research journals for publishing hydrogen storage using HEA is shown in Fig. 4. The map was created using a minimum of two article publications along with at least two citations using the VOSviewer software. It should be highlighted that bibliometric literature has no standardized criteria of a network map of this kind.

About 20 journals that consequently met the above-mentioned criteria. Table 1 shows the ranking of the top 20 Journals based on number of publications, total links and citations. The total link strength

is a metric utilized to assess the overall strength of the connections between a given item (e.g., author, journal, etc.) and other items that are being studied. Fig. 4 has 10 clusters of journals which are indicated by different colours. Journal with the same cluster illustrate high co-citational than other journals in different clusters. The node assigned to a journal indicates the journal's influence in terms of number of publications (or citations). The strength of two journals is determined by the length of their link line, the shorter the line the stronger their relationship. The most preferred journal as seen in Table 3 is the international journal of hydrogen energy with a total link strength of 243, 42 publications and highest citation with 1607 citations. This is followed by Journal of alloys and compounds (23 publications and 536 citations), inorganic chemistry (3 publications and 202 citations) and Scripta Materialia (5 publications and 255 citations) making the top four. There is no clear relationship between publications and number of citations, however quality of research work, novelty, journal publication model along with reputation of journal have aided in gaining citations.

3.3. Scientific collaboration networks

3.3.1. Analysis of co-authorship of researchers

Collaboration is a key element within the research community enabling knowledge sharing and technological transfer. This helps researchers gain access to expensive and specialized research facilities along with the ability to interact with experts within the field of interest. Co-authorship cluster density maps of authors were generated using VOSviewer. The criteria used to identify the top authors in the subject of high-entropy alloys for hydrogen storage were a minimum number of documents of an author set at nine, whereas the minimum number of citations of an author was kept at two. Fig. 5 shows a density cluster map of the top 10 researchers on high-entropy alloys for hydrogen storage. The top 10 authors are based on total link strength and additional criteria seen in Table 2. The grouping of researchers based on clusters signifies collaborating groups. Researchers in each cluster represent a collaborating group.

The top 5 authors based on publications are Zlotea C (16 articles), Zepon G (16 articles), Edalati K (12 articles), Sahlberg M (11 articles), and Ek G (11 articles). The number of publications, however, does not correlate to citations as the Top 5 most cited authors differ from that of the Top 5 publishing authors. Top 5 cited authors are Sahlberg M (809 citations), Zlotea C (669 citations), Ek G (571 citations), Zepon G (525 citations), and Edalati K (411 citations), respectively. The comparison of Top 5 publishing and Top 5 cited authors shows that high publications do not necessarily result in high citations. High citations can be contributed by factors such as novelty, reputation of the publishing journal, quality of work, along with the access type.

3.3.2. Analyses of institutional and international co authorship

The analysis of co-authorship from various institutions is given Table 3. The criteria are based on at least four publications with 11 of citations. Ten out of 367 organizations met these criteria which are the top 10 institutions focusing on HEA-based hydrogen energy and storage investigations. Out of the 10 institutions only seven have collaborative links with other institutions showing relatively low inter-institutional collaboration. The Institute of Nuclear Physics and Chemistry of China has the highest number of publications with 11 articles published, whereas the International Institute for Carbon Neutral Energy Research in Japan has the highest number of citations at 368 citations. Although, the Institute of Nuclear Physics and Chemistry has more publications but does not have the highest number of citations. This can be due to various reasons such as journal reputation, quality of work and open access.

The total link strengths of the institutions involved in this research are relatively low. Total link strength reflects the degree of co-authorship between institutions, suggesting that most of these entities have minimal collaboration with each other. In Table 3, more than half of the contributing institutions are based in China, based on the total

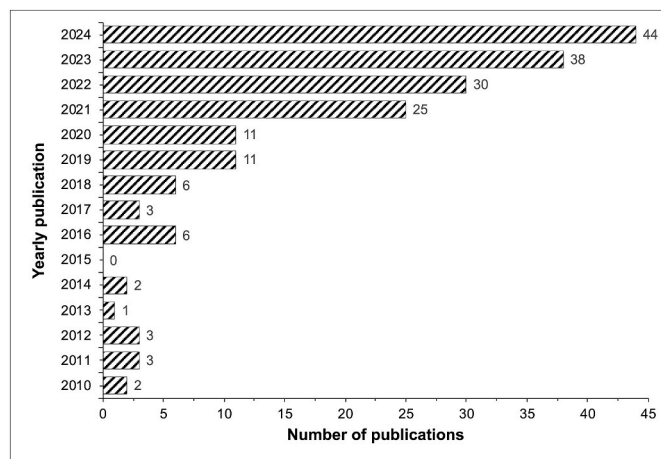


Fig. 3. Annual distribution of publications focusing on hydrogen storage of HEAs/CCAs based on Scopus Database.

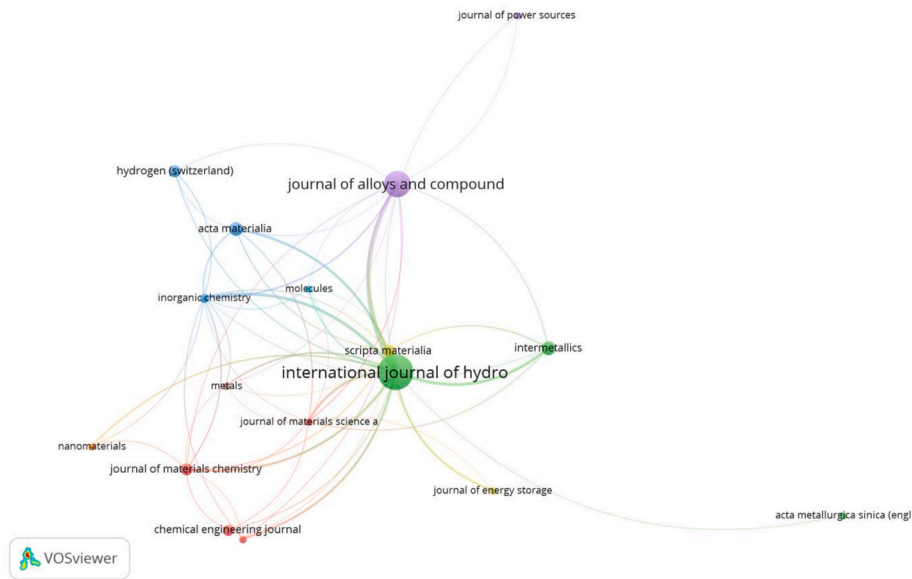


Fig. 4. Top journals focusing on hydrogen storage publications.

Table 1
Top 20 journals focusing on hydrogen storage research.

No	Journal	Cluster	No of articles	Citations	Links	Total link strength
1	International Journal of Hydrogen Energy	3	42	1607	16	243
2	Journal of Alloys and Compounds	5	23	536	12	95
3	Inorganic Chemistry	2	3	202	12	61
4	Scripta Materialia	4	5	255	10	61
5	Journal of Material Chemistry A	1	5	27	9	36
6	Intermetallics	3	6	36	5	34
7	Journal of Materials Science and Technology	1	2	112	10	33
8	Acta Materialia	2	6	236	6	32
9	Renewable Energy	1	2	26	6	22
10	Metals	6	2	15	6	16
11	Journal of Energy Storage	4	2	5	3	11
12	Nanomaterials	8	2	134	3	10
13	Molecules	11	4	32	5	9
14	Chemical Engineering Journal	1	5	46	4	8
15	Hydrogen (Switzerland)	2	2	25	4	8
16	Journal of Power Sources	5	2	53	2	2
17	Acta Metallurgica Sinica	3	2	13	1	1
18	Journal of Iron and Steel Research International	7	2	21	0	0
19	Journal of Physics and Chemistry of Solids	9	2	17	0	0
20	Xiyu Jinshu Cailiao Yu Gongcheng/Rare Metals Materials and Engineering	10	2	6	0	0

number of research publications. To advance this field, fostering international and inter-institutional collaboration is crucial. This can be achieved through knowledge sharing and technology transfer.

The density map of countries with the highest number of publications, created using VOSviewer is given in Fig. 6. The parameters set for this analysis included a minimum of three documents and three citations per country. The analysis revealed that 35 countries focus on hydrogen storage using HEAs, but only 18 meet the criteria. South Africa and Nigeria, with one publication and three citations respectively, are the only African nations contributing to this field; however, they are excluded as they do not meet the threshold. On the density map, the brighter and larger the node, the greater the number of publications attributed to that country. China, with 85 articles, has the largest and brightest node, followed by Brazil (23 articles) and France (21 articles). The map indicates established international collaboration among countries working on hydrogen energy development and storage materials.

The Top 10 publishing countries in the field of hydrogen energy storage using HEAs/CCAs is given in Table 4. China leads the list with a significant number of publications (85) and a high citation count (1500), indicating substantial research activity in this area. Brazil and France follow closely in terms of publication output. Notably, Sweden and Norway, despite having fewer publications compared to China, exhibit high citation counts, suggesting their research has a considerable impact on the field. These valuable insights into the global research landscape highlight the prominent role China continue to play and the significant contributions from other countries like Brazil, France, and the Nordic nations.

3.4. Citations analysis of most influential articles on hydrogen storage using HEA

The citations analysis of the most influenced articles on hydrogen storage using high entropy alloys is given in Fig. 7. The outcomes of the analysis of the most influential publications are presented in this section. The minimum number of citations to generate the figure on VOSviewer was 20 citations and only 60 publications out of 171 articles. These 60 articles are shown in Fig. 7. The highest cited article on HEAs for hydrogen storage is Sahlberg et al. with 241 citations, followed by Kunce, Polanski & Bystrzycki with 193 citations and Kao et al. (pioneer) with 191 citations. Kunce, Polanski & Bystrzycki with 189 citations and Zlotea et al. with 147 citations complete the Top 5 in this field. Further

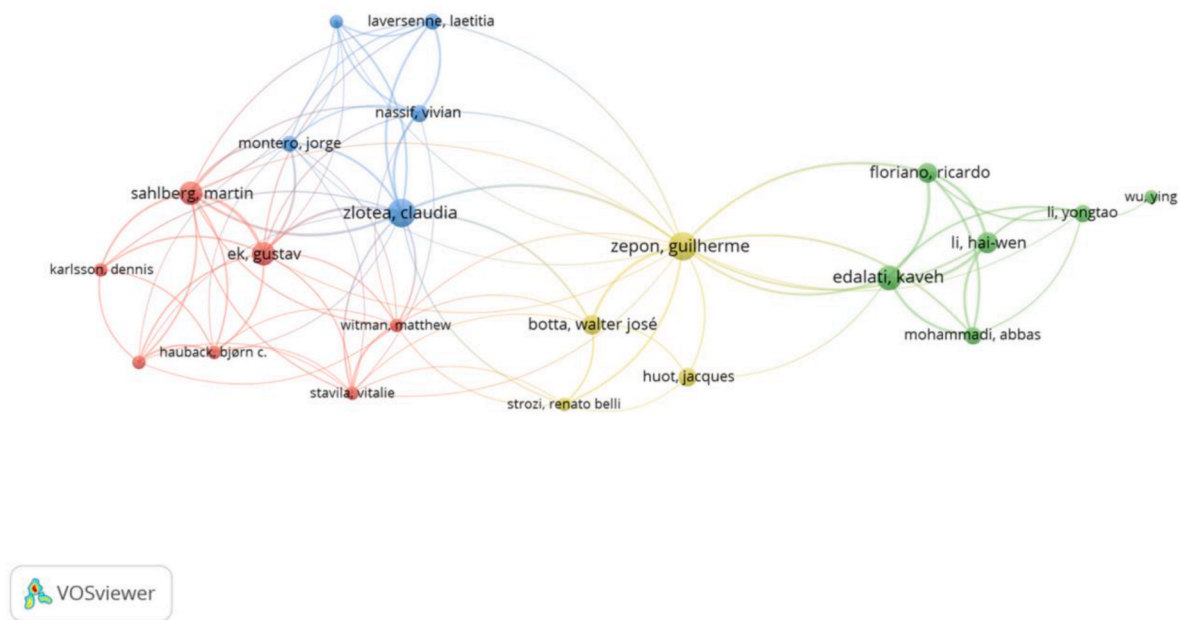


Fig. 5. Co-authorship of researchers.

Table 2
Top 20 publishing authors.

No	Author	Cluster	No. of articles	Citations	Institution/Country
1	Zlotea C	1	16	669	East Paris Institute of Chemistry and Materials
2	Zepon G	1	16	525	Universidade Federal de Sao Carlos
3	Edalati K	3	12	411	Kyushu University
4	Sahlberg M	1	11	809	Uppsala university
5	Ek G	1	11	571	Uppsala university
6	Li H	3	9	399	Hefei General Machinery Research Institute
7	Hu J	2	9	293	University of electronic Science and Technology of China
8	Shen H	2	9	293	China Academy of engineering Physics
9	Xiao H	2	9	293	University of electronic Science and Technology of China
10	Zu X	2	9	293	University of electronic Science and Technology of China

details pertaining the most cited articles and publications are outlined in Table 5.

Although the work on the TiVZrNbH metal hydride by Sahlberg et al., significantly advanced the field, they were not the first to pioneer HEA metal hydrides; that distinction belongs to Kao et al., who initially introduced HEA metal hydrides based on the CoFeMnTiVZ system. However, Sahlberg et al. attracted substantial attention by developing an HEA alloy with hydrogen-to-metal (H/M) ratio of 2.5, surpassing previously reported storage capacities in HEA-based metal hydrides. Furthermore, the BCC phase of the TiVZrNbH alloy set the foundation for further research into BCC-based HEA metal hydrides for hydrogen storage applications. Meanwhile, Kunc et al.'s work extended beyond HEA metal hydrides by providing a robust framework for fabricating HEAs through Laser Engineering Net Shaping (LENS), thereby broadening the appeal and application of their research. Additionally, Zlotea et al. demonstrated that the TiZrNbHfTa alloy exhibited single-step

Table 3
Top publishing institutions focusing on hydrogen storage HEA research.

No	Institution	Country	No of articles	Citations	Total link strength
1	Institute of Nuclear Physics and Chemistry	China	11	301	9
2	WP International Institute for Carbon Neutral Energy Research	Japan	10	368	6
3	Central Iron and Steel Research Institute	China	10	122	0
4	University of Electronic Science and Technology	China	9	210	9
5	University of Campinas	Brazil	4	126	5
6	Nefei General Machinery Research Institute	China	4	91	5
7	Sandia National Laboratories	USA	4	85	0
8	University Grenoble Alpes	France	4	44	0
9	Shandong University of Science and Technology	China	4	39	4
10	Harbin Institute of Technology	China	4	39	4

hydrogen absorption along with high storage capacity, a performance attributed to significant lattice distortion, a core effect underpinning hydrogen storage in later investigations. The innovative features in these studies have collectively fuelled ongoing interest and explain the high citation rates associated with their publications.

3.5. Co-occurrence network of all keywords

A co-occurrence network provides valuable insights into major research areas and emerging topics. Using VOSviewer, a co-occurrence map of author keywords was generated with a minimum occurrence threshold of five. Out of 1291 keywords, 139 met this criterion. In Fig. 8, each node represents a keyword, with node size proportional to its frequency, and distances reflecting the strength of association between terms. Keywords sharing the same colour are grouped into clusters, indicating higher co-occurrence rates. Seven clusters were identified. The largest, highlighted in red, includes "hydrogen storage" (210

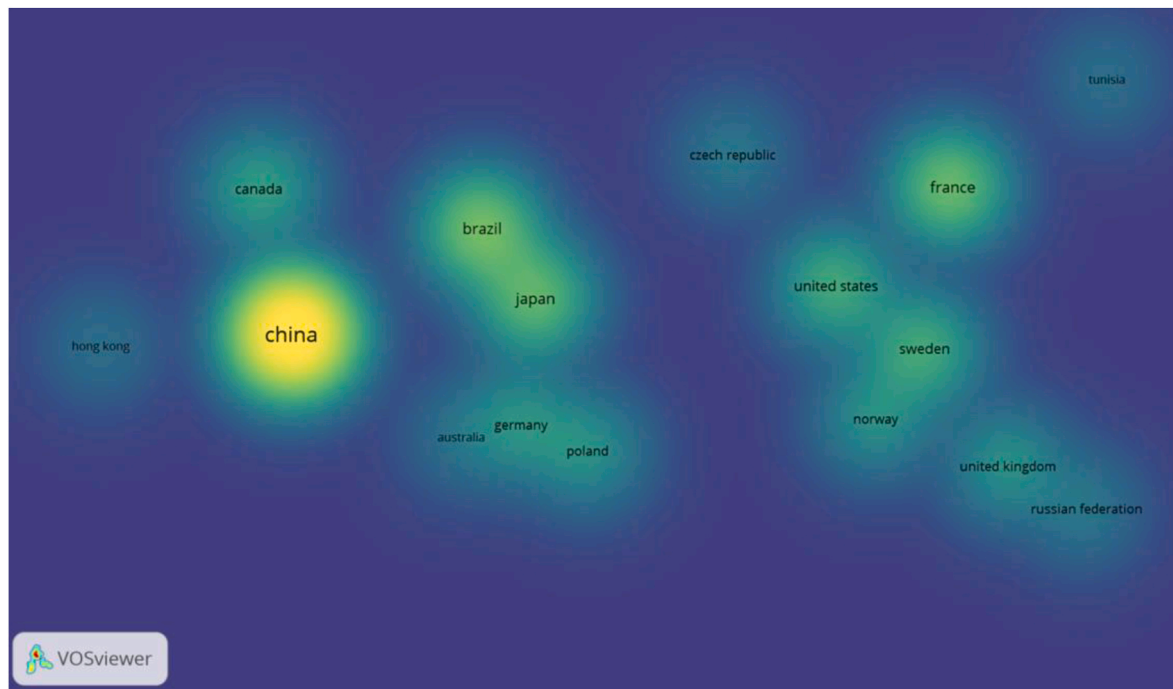


Fig. 6. Leading countries on HEA hydrogen storage research.

Table 4

Top publishing countries focusing on hydrogen energy storage using HEAs/CCAs.

No	Country	Number of articles	Citations
1	China	85	1500
2	Brazil	23	853
3	France	21	895
4	Japan	19	665
5	Sweden	14	969
6	United states of America	14	621
7	Canada	11	240
8	Poland	8	489
9	Norway	8	431
10	Germany	8	157

occurrences, 126 links) and "high entropy alloys" (152 occurrences, 118 links), along with "hydrides," "titanium alloy," and "entropy." The second cluster, shown in green, centres on "hydrogen storage alloys" (74 occurrences) and includes terms such as "hydrogen absorption," "activation energy," and "thermodynamics," emphasizing hydrogen storage properties and alloy systems.

The third cluster, shown in blue, features keywords such as "hydrogen" (26 occurrences, 92 links), "hydrogen absorbing materials," "X-ray diffraction," and "metal hydrides." The fourth cluster, highlighted in yellow, includes "iron alloys" (49 occurrences, 117 links), "chromium alloys," "cobalt alloys," "multi-principal element alloys," and "storage performance." The fifth (purple), sixth (light blue), and seventh (orange) clusters focus on terms like "hydrogen storage capacities," "hydrogen storage behaviors," "hydrogen storage materials," "hydrogen sorption," and "arc melting." The overall bibliometric results indicate that hydrogen storage research using CCAs/HEAs remains a relatively young field compared to other solid-state methods. Notably, keywords related to alloy systems (e.g., titanium, cobalt, chromium, iron) and lattice structures (BCC and Laves phases) emphasize their critical influence on hydrogen storage capacity and kinetics.

Manufacturing route is underlined in the keywords as denoted by keywords such as arc melting and high ball milling, the processing route plays a role in how microstructure and subsequently the crystal structure

of an alloy system is which will affect the hydrogen storage properties of a particular alloy system.

Keywords such as CALPHAD (calculation of phase diagrams) and thermodynamics assist in designing HEAs. Hydrogen storage properties dominated keywords in Fig. 8 with words such a hydrogen storage, hydrogen storage capacity, hydrogen storage kinetics, activation energy and hydrogen absorption to name a few being highlighted in the keywords. These keywords are of importance as the illustrate the hydrogen storage capabilities of a HEA alloy system, these properties can be tested using a PCT (pressure composition temperature) test which is also known as a PCI (pressure composition isotherm) test which is also denoted in the keywords.

Majority of studies focusing on hydrogen storage using HEA focus on the hydrogen storage properties especially the hydrogen storage capacity as HEA alloys can store hydrogen at room temperature which is unique in terms on solid state hydrogen storage [70]. Mechanism which leads to hydrogen storage properties have not been researched as denoted by the small nodes on crystal structure, microstructure and thermodynamic keywords, this highlights that research can still be done in this particular area. Processing route is another area of hydrogen storage using HEA that can be further researched as denoted by the small nodes on arc melting and high balling.

It is of importance to bear in mind that other keywords have been excluded from the analysis as they have not met the minimum threshold of 5. Keywords such a computer model (1 occurrence), commercial applications (1 occurrence), refractory high entropy alloys (1 occurrence) and laves phase hydrides (1 occurrence). The occurrences that do not meet the threshold indicate a potential for future research work in this field.

3.6. Insights from the bibliometric review

The bibliometric analysis shows a consistent increase in publications on CCAs/HEAs for hydrogen storage since 2010. This reflects the growing global emphasis on clean energy which aligns with Sustainable Development Goal 7 (Affordable and Clean Energy). China emerges as the leading contributor, with a few other countries playing significant roles in research output and collaboration. However, limited inter-

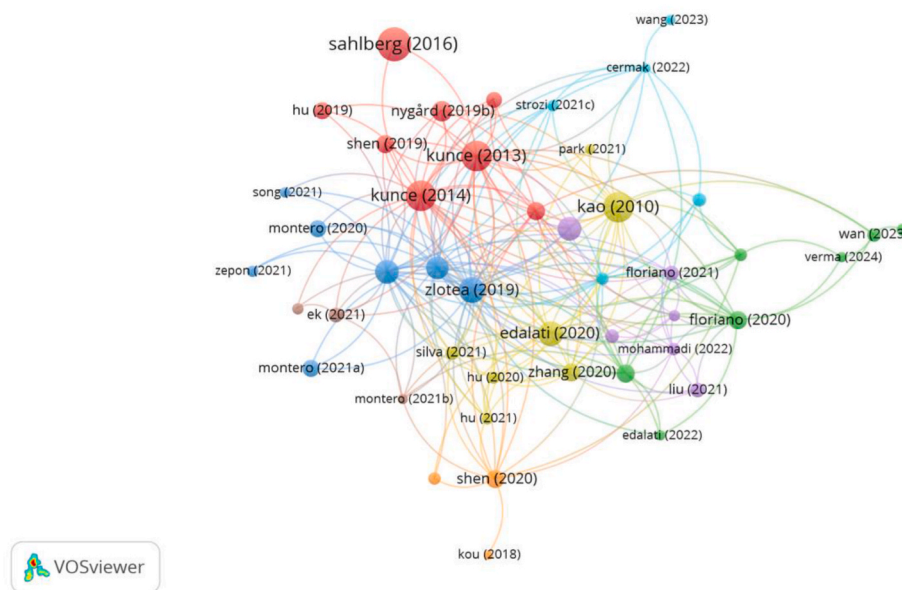


Fig. 7. Distribution of most cited journal articles.

institutional cooperation suggests untapped potential for broader global partnerships to enhance knowledge exchange and accelerate industrial adoption. The use of VOSviewer to map keyword co-occurrence provided insights into dominant research themes such as “BCC structure,” “Laves phase,” and “hydrogen absorption” highlighting key focus areas. Despite this, gaps remain in understanding microstructural influences, thermodynamic stability, and lattice behavior, which are essential for optimizing hydrogen storage performance in HEAs.

The bibliometric review critically evaluates current methodologies and the inherent limitations. The main one is the particular reliance on Scopus and English-language sources, which may exclude relevant international studies. Addressing this would improve the comprehensiveness of future bibliometric assessments. Importantly, the role of computational modeling and machine learning in accelerating HEA development by predicting hydrogen capacity and guiding composition design is emphasized. However, the effectiveness of these tools is constrained by limited datasets and the complexity of underlying material behaviours. Expanding data availability and improving algorithm robustness are therefore crucial next steps. By synthesizing structural, computational, and bibliometric insights, a roadmap is provided for advancing HEA/CCA-based hydrogen storage and underscores the need for interdisciplinary strategies to translate innovation into practical renewable energy solutions.

3.7. Limitations of bibliometric study

Bibliometric analysis has some drawbacks. Firstly, it only used Scopus for literature search, potentially missing important articles not included in this database. Future research could benefit from searching multiple databases to ensure a more thorough coverage of relevant literature. Secondly, the focus solely on English language articles may overlook valuable insights published in other languages. Expanding the language criteria could make the analysis more inclusive. Lastly, the exclusion of sources like conference proceedings, books, and encyclopedias limits the breadth and depth of analyses. Incorporating these sources in future studies could enrich the findings.

4. Review of hydrogen storage and applicable materials

Hydrogen fuel is one of the renewable sources of energy for the drive towards sustainable development goal (SDG 7). Hydrogen is an energy

carrier, able to storage energy and can be used as chemical feedstock and has the potential for decarbonization, clean energy solution to mitigate climate change, high energy density than lithium-based fuel cells, could replace natural gas in gas turbines and able to promote zero emission transport [13,21,31,33,71]. Fig. 9 provides a classification of hydrogen fuels based on their sources, production processes, and their potential for decarbonization. Each colour designation represents a distinct production method and its environmental impact. Green hydrogen is produced via water electrolysis using renewable energy with the most sustainable with zero carbon emissions. Blue hydrogen relies on fossil fuels and incorporates carbon capture and storage to reduce emissions. Grey hydrogen is mainly extracted from natural gas from steam-methane reforming and carbon-intensive without mitigation. Pink or purple hydrogen uses nuclear power for electrolysis, offering low-carbon production depending on the sustainability of nuclear energy. Turquoise hydrogen comes from methane pyrolysis mainly producing solid carbon instead of CO₂ and largely dependent on fossilized methane. Brown/black hydrogen, derived from coal gasification, has a high carbon footprint due to CO₂ emissions. Yellow hydrogen represents a hybrid approach using grid electricity, while white hydrogen is a by-product of industrial recycling processes. This categorization highlights the diversity of hydrogen production pathways and their alignment with decarbonization goals.

4.1. An overview of approaches for hydrogen storage

One of the effective pathways of storing solid hydrogen is by material-based methods. These include the use of adsorbent, liquid organic systems, interstitial hydrides, complex hydrides and chemical hydrogen. The various classes of conventional materials being used for hydrogen storage with main shortcoming are summarized in Fig. 10. However, the recent material design based on high entropy and complex concentrated alloys paved way for structural and functional applications. Thus, HEAs/CCAs are being rigorously studied for hydrogen storage applications.

4.2. Compositionally complex alloys and hydrogen storage

Complex concentrated alloys (CCAs) are the broad class of multiple principal element-based materials. Generally, CCAs fall within the domain of equiatomic and non-equiatomic amounts with no restrictions

Table 5

Top articles on HEA for hydrogen storage.

No	Article title	Journal	Citations
1	Superior hydrogen storage in high entropy alloys	Scientific Reports	241
2	Microstructure and hydrogen storage properties of a TiZrNbMoV high entropy alloy synthesized using Laser Engineered Net Shaping	International Journal of Hydrogen Energy	193
3	Hydrogen storage properties of multi-principal-component CoFeMnTiVZr alloys		191
4	Structure and hydrogen storage properties of a high entropy ZrTiVCrFeNi alloy synthesized using Laser Engineered Net Shaping		189
5	Hydrogen sorption in TiZrNbHfTa high entropy alloy	Journal of alloys and compounds	147
6	Reversible room temperature hydrogen storage in high-entropy alloy TiZrCrMnFeNi	Scripta Materialia	135
7	Counting electrons - A new approach to tailor the hydrogen sorption properties of high-entropy alloys	Acta Materialia	118
8	Structure and Hydrogenation Properties of a HfNbTiVZr High-Entropy Alloy	Inorganic chemistry	117
9	Hydrogen-induced phase transition of MgZrTiFe _{0.5} Co _{0.5} Ni _{0.5} high entropy alloy	International Journal of hydrogen energy	112
10	Hydrogen storage in high-entropy alloys with varying degree of local lattice strain		86
11	Analysis of phase formation in multi-component alloys	Journal of Alloys and Compounds	77
12	High-Entropy Alloy with Mo-Coordination as Efficient Electrocatalyst for Oxygen Evolution Reaction	ACS Catalysis	76
13	Study on the hydrogen storage properties of a TiZrNbTa high entropy alloy	International Journal of Hydrogen Energy	71
14	Synthesis and hydrogen storage behavior of Mg-V-Al-Cr-Ni high entropy alloys		71
15	Hydrogen storage in TiZrNbFeNi high entropy alloys, designed by thermodynamic calculations		70
16	A Novel TiZrHfMoNb High-Entropy Alloy for Solar Thermal Energy Storage	Nanomaterials	70
17	Compositional dependence of hydrogenation performance of Ti-Zr-Hf-Mo-Nb high-entropy alloys for hydrogen/tritium storage	Journal of Material Science and Technology	69
18	Microstructures and hydrogen storage properties of La-Ni-Fe V-Mn alloys	International Journal of Hydrogen Energy	66
19	Hydrogen storage properties of the refractory Ti-V-Zr-Nb-Ta multi-principal element alloy	Journal of Alloys and Compounds	64
20	A DFT study in hydrogen storage in high entropy alloy TiZrHfScMo	Nanomaterials	64

on the composition and with at least three elemental compositions. It is the deviation from the initial assumption of the ideal theory of high entropy alloy formation. The high entropy alloys are a subset of CCAs with stringent equiatomic proportions of five constituent elements ranging from 5 to 35 at% [18]. The foundational theory behind HEAs is the maximization of configurational entropy to stabilize the formation of disordered single-phase solid solutions (SS), which can adopt FCC_SS, BCC_SS, or HCP_SS structures [25,72–78]. This emphasis on entropy-stabilized phases led to the exploration of the central region of the hyper-dimensional phase diagram in the late 1990s and early 2000s [18,79], whereas the broader compositional spaces of higher-order systems remained largely underexplored until. Thus, CCAs or multi-principal element alloys (MPEAs) highlight the vast compositional space, independent of phase types or configurational entropy levels

[80]. The medium entropy alloys (MEAs) composed of three to four elements constituents. The distinguishing features of this class of alloys is the idea of no single element dominating the composition as observed in dilute alloys [81]. A schematic showing the relationship and the differences between CCAs, HEAs and MEAs is presented in Fig. 11.

Alloy design strategies in multicomponent systems are fundamentally guided by free energy as a function of composition. In an ideal high-entropy regime, where three elements are combined at or near equiatomic ratios (Fig. 12), the configurational entropy is maximized [18, 83–86]. This leads to a lowering of the Gibbs free energy curve sufficiently to stabilize a single-phase solid solution, as depicted in the upper right schematic [87–92]. In this scenario, the constituent elements are randomly distributed within a common lattice, minimizing the chemical potential differences [93–98]. This strategy is typically targeted in traditional HEA design to achieve structural homogeneity and enhanced functional properties such as hydrogen storage reversibility and diffusion kinetics.

A deviation from the ideal entropy-driven scenario can give rise to multiple solid solutions, as shown in the lower left of Fig. 12 [24]. Here, while high entropy still plays a stabilizing role, the enthalpy of mixing between certain element pairs may become sufficiently unfavourable to induce phase separation into distinct solid solution regions. For a three-element system, this may manifest as two or three coexisting phases, each enriched in different principal elements, but retaining solid solution character rather than forming ordered intermetallic compounds. This strategy leverages partial segregation to optimize mechanical and diffusion properties, potentially creating tailored hydrogen trapping sites or diffusion pathways.

Further reduction in the stabilizing effect of configurational entropy, combined with significant enthalpic driving forces, can lead to the formation of intermetallic phases coexisting with solid solutions as shown in the lower right schematic. In a three-element system, this could correspond to the precipitation of ordered compounds between two elements, embedded within a matrix of a remaining solid solution. Such structures often exhibit superior strength but can compromise hydrogen storage properties due to the brittle nature of intermetallics. However, careful control over phase volume fractions and distribution can mitigate these drawbacks, providing a design pathway that balances structural integrity and hydrogen absorption capacity.

Finally, in highly concentrated systems where enthalpic interactions dominate over configurational entropy, spinodal decomposition may occur, as shown in the upper left diagram. In a three-component equiatomic alloy, small compositional fluctuations spontaneously grow without nucleation barriers, leading to a finely modulated, compositionally distinct microstructure. Spinodal decomposition can severely impact hydrogen diffusion by creating complex pathways and local chemical inhomogeneities. Nevertheless, in controlled scenarios, such as nanostructured materials, it may be harnessed to enhance hydrogen sorption kinetics through increased interface density. Thus, understanding and controlling the free energy landscape is crucial for designing advanced CCAs and HEAs optimized for solid-state hydrogen storage.

The classification of the alloys from the entropic contribution is from statistical mechanics and based on the Boltzmann's hypothesis [80,96, 98]. This relates the configurational entropy and the mixing complexity as a function of the molar gas constant (R). The low entropy alloy as a function of molar gas constant is given as $\Delta S_f \leq R$; MEAs ($R < \Delta S_f \leq 1.5R$) and HEAs ($\Delta S_f > 1.5R$) [80,96,98].

The applications of HEAs/CCAs fall under two main groups. These are the structural and functional applications which are summarized in Fig. 13. The “structural” category is characterized by high strength, ductility, toughness, fracture toughness, wear resistance, radiation resistance, and resistance to softening and creep. The “functional” category highlights the potential in various applications, including magnetocaloric effect, biomaterials, shape memory effect, superconductivity, high saturation magnetization, high electrocatalytic activity,

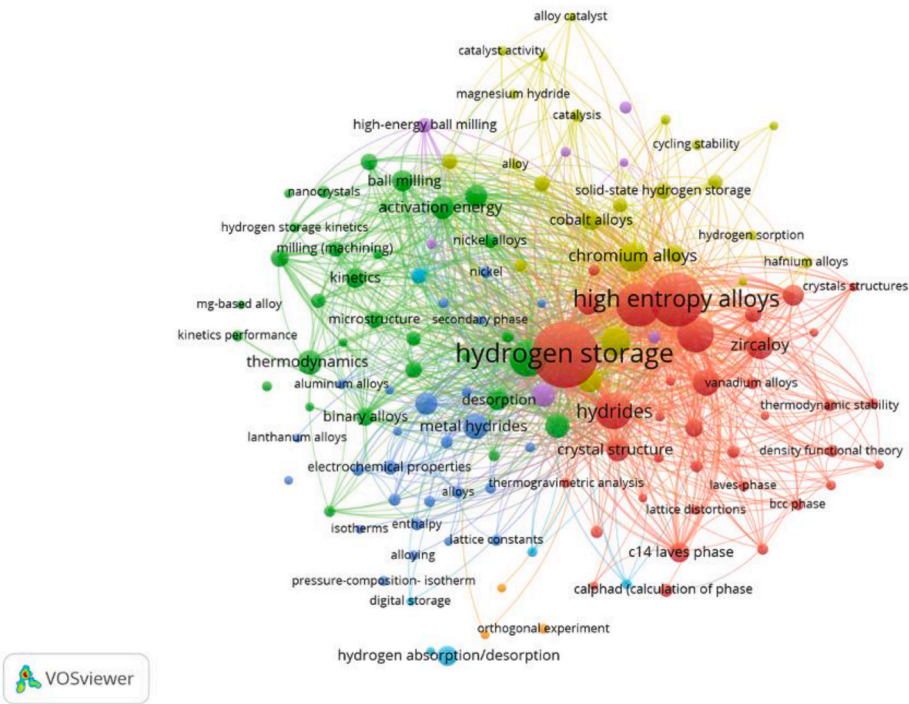


Fig. 8. Prominent keywords highlighting areas of importance and exploring some gaps.

Colour designation	Source of production, processes and the decarbonization for domestic and industrial applications
Green	Produced from electrolysis of water using electricity from renewable energy, i.e., solar or wind. Zero emission of Carbon dioxide
Blue	Produced from fossilized fuel sources Produces CO ₂ , which can be captured, repurposed or stored
Grey	Extracted from natural gas using steam-methane reforming
Purple / pink	Produced from electrolysis using nuclear power
Turquoise	Produced from thermal splitting of methane (pyrolysis)
Brown / black	Coal gasification with massive emission of CO ₂
Yellow	Electrolysis of water using grid electricity from renewables & fossil fuels
White	By-product of industrial process - process of recycling

Fig. 9. Different hydrogen energy sources which is associated with colour based on production routes.

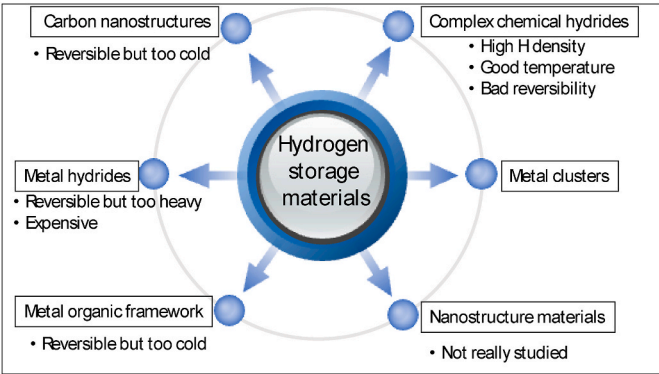


Fig. 10. Main conventional materials for hydrogen storage with shortcomings.

catalytic reactivity and stability and high hydrogen storage capacity. The wide range of applications are primarily due to expansive compositional flexibility, diverse microstructures, and robust underlying mechanisms (Fig. 14). Furthermore, integrating mechanistic alloy design criteria especially mechanical and chemical metastability into fundamental HEA/CCA concepts has led to the emergence of multiple alloy classes that combine both functional and structural properties [24]. Thus, one can use high entropy concepts to shift compositions into thermodynamically stable regime to trigger specific, designed and desired mechanisms other than just solid solution as shown in Fig. 14 [24].

The structural and chemical complexity of CCAs/HEAs make them attractive for hydrogen-related applications. These include hydrogen storage, which demands high capacity and favourable thermodynamics, and structural components resistant to hydrogen embrittlement [99–107]. Their vast compositional space enables property tuning, while chemically diverse and distorted lattices offer advantages over

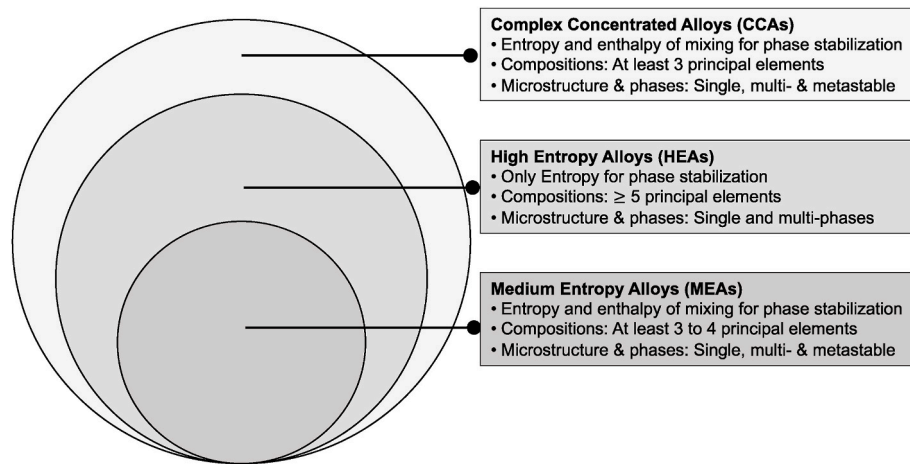


Fig. 11. Schematic diagram showing the classes of complex concentrated alloys based on compositions [82].

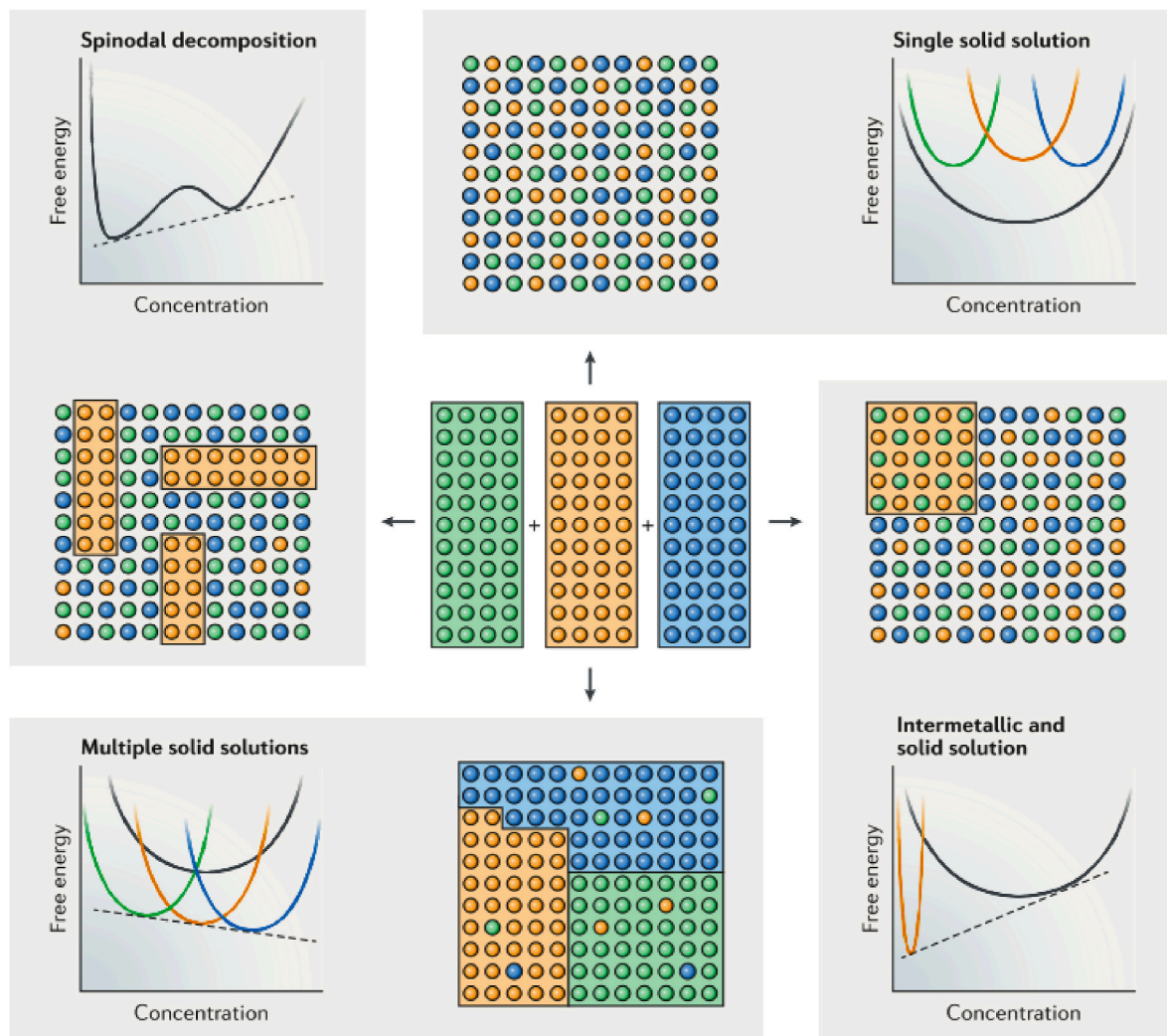


Fig. 12. Schematic illustration of phase formation strategies in multicomponent alloys based on free energy and concentration relationships. The diverse microstructural evolution pathways accessible in CCAs and HEAs through controlled compositional design [24].

conventional metals [108]. Variations in local atomic environments yield a spectrum of hydrogen binding energies, allowing tailored absorption/desorption behavior or trapping sites that reduce embrittlement [109]. Severe lattice distortion can enhance hydrogen

accommodation by opening interstitial sites inaccessible in simpler lattices [110]. Understanding how multi-elemental compositions influence electronic structure and hydrogen bonding is essential for optimizing CCAs/HEAs for hydrogen storage applications. This is a function of the

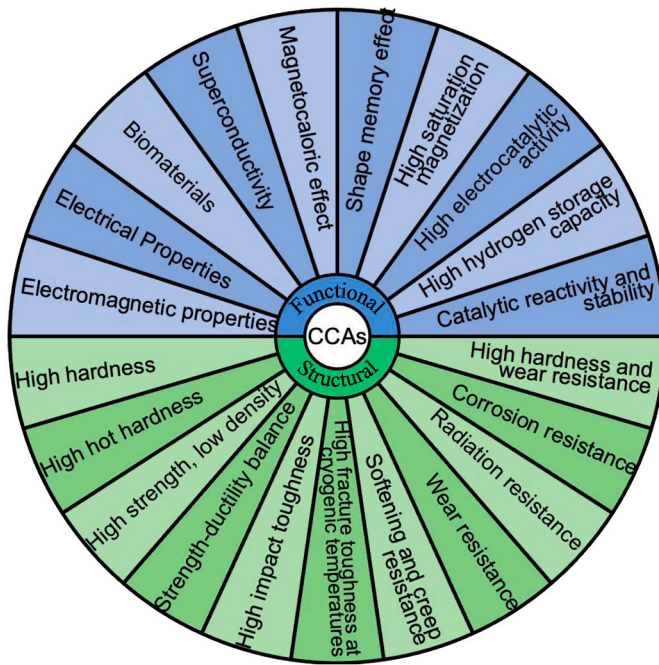


Fig. 13. Summary of the structural and functional applications of CCAs/HEAs.

four core effects which are the maximization of the configurational entropy effect, severe lattice distortion, sluggish diffusion, and the cocktail effect as shown in Fig. 15 [67] with the schematic representation in Fig. 16 [111]. The interrelated between the core effects to the underpinning sciences and how it provides insights to the physical metallurgy of HEAs is highlighted.

4.2.1. Multiple elements, local chemical variation and hydrogen uptake

Configurational entropy plays a crucial role in the thermodynamics of HEAs and CCAs. Their unique compositions, typically comprising multiple principal elements, result in high configurational entropy [24, 72,83,113–123]. This stabilises simple solid-solution phases such as FCC, BCC, or HCP over complex intermetallic phases [15,93–95,97,98, 124]. This stabilization occurs through a reduction in Gibbs free energy ($\Delta G = \Delta H - T\Delta S$), as the high configurational entropy contributes significantly more in most HEAs than in conventional alloys [125].

The macroscopic thermodynamic properties governing hydrogen absorption and desorption in CCA/HEA systems are intrinsically linked to the electronic structure and hydrogen–metal bonding characteristics. Key parameters include the enthalpy of solution/formation (ΔH) [125, 126], which quantifies the heat released or absorbed when hydrogen dissolves into the metal lattice or forms a hydride [112,127–132]. A negative ΔH indicates exothermic, favourable hydrogen binding, with more negative values implying stronger binding and requiring higher desorption temperatures, whereas values near zero correspond to weaker binding and easier release [3,53,126,128,129,112,131]. The entropy of solution/formation (ΔS) reflects the change in disorder, primarily due to the loss of configurational entropy of H_2 gas, typically resulting in negative ΔS , with additional contributions from vibrational entropy [3,21,23,29,59,127,131]. The Gibbs free energy governs the spontaneity of hydrogen absorption/desorption at a given temperature and pressure, with equilibrium defined by $\Delta G = 0$, as per the van't Hoff equation [128,133–136]. Additionally, the binding energy (EB), often determined computationally, represents the energy required to remove a hydrogen atom from a specific interstitial site and closely correlates with ΔH [126].

The compositional randomness inherent in HEAs/CCAs reduces the probability of atomic pair formation, further enhancing entropy-driven phase stability. This high configurational entropy is fundamental to the superior phase stability and mechanical properties observed in HEAs (Fig. 16(a)) [111]. It arises from the incorporation of multiple principal elements, providing robust thermodynamic stability and preventing the formation of brittle intermetallic phases even at elevated temperatures.

The high entropy effect is particularly beneficial for hydrogen storage applications. It facilitates the formation of solid-solution BCC phases, which are more favourable for hydrogen absorption due to their abundance of interstitial sites [137,138]. Specifically, BCC structures inherently provide a greater number of energetically favourable tetrahedral interstitial sites compared to FCC or HCP lattices, offering higher hydrogen occupancy [65]. Additionally, the high-entropy effect generates numerous defects within the crystal lattice, such as voids and interstitial spaces, which act as potential sites for hydrogen absorption, thereby significantly enhancing the overall hydrogen storage capacity of the alloys [139].

In CCAs/HEAs, the random or quasi-random arrangement of multiple metal atoms creates highly variable local chemical environments around each potential interstitial site [109]. For instance, a hydrogen atom in a tetrahedral site may be surrounded by different combinations of elements (e.g., 2 Ti, 1 V, 1 Zr vs. 1 Ti, 2 V, 1 Nb), influencing hydrogen

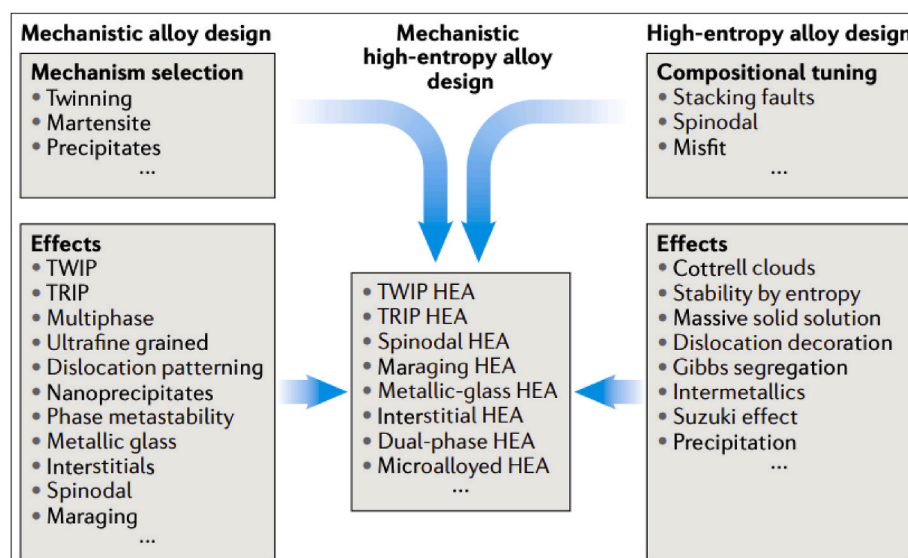


Fig. 14. Exploring the interplay between mechanistic design and compositional tuning in the development of advanced HEAs [24].

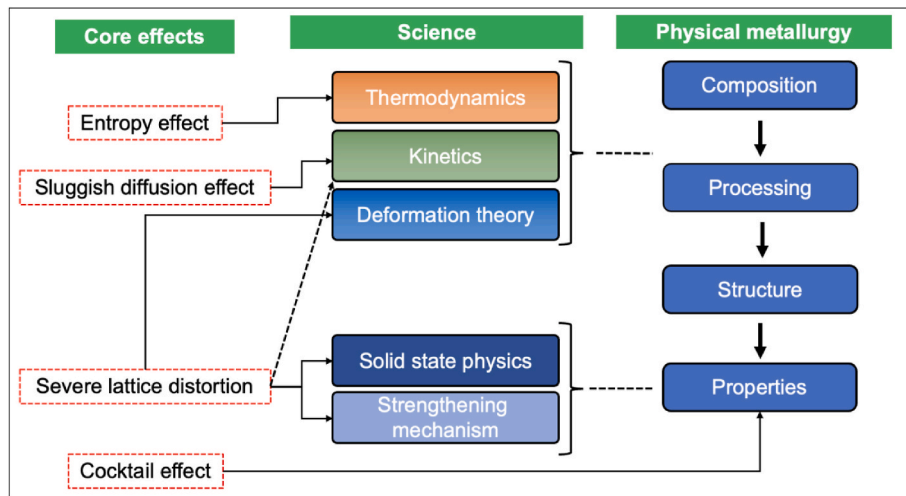


Fig. 15. Four core effect driving the structural and functional properties of HEAs/CCAs [98].

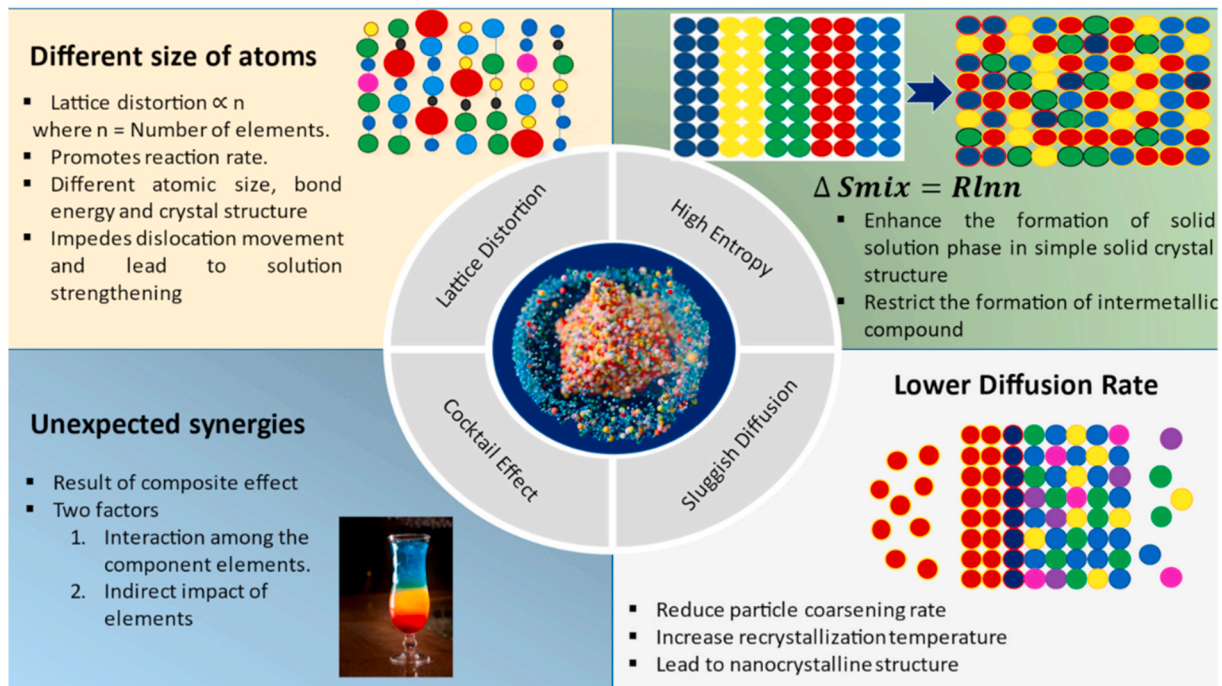


Fig. 16. Schematic representative of four core effects and the role in the design of HEAs/CCAs [111].

interactions. This variation leads to a distribution of hydrogen binding energies (EB), rather than a single value as seen in pure metals [35,112,131,132,140]. Some environments bind hydrogen more strongly (more negative EB or ΔH), while others bind it weakly. This distribution stems from the intrinsic chemical and structural disorder and requires statistical modeling. Inelastic neutron Scattering (INS) supports this, revealing broadened vibrational peaks indicative of a range of M – H bond strengths and distances [109].

The specific chemical nature of neighbouring metal atoms significantly influences the local electronic structure at interstitial sites. Variations in electronegativity and the availability of valence orbitals for hybridization affect charge transfer and the strength of covalent interactions between hydrogen and surrounding metals [126]. Thus, DFT studies are essential for probing these local effects. In TiZrHfScMo, DFT calculations show hydrogen 1s orbitals primarily hybridize with the s orbitals of nearby metal atoms, with projected density of state (PDOS) and overlap population analyses revealing strong covalent M – H

bonding [126]. Element-specific charge transfer occurs during hydrogenation: Ti and Sc lose electron density, while Mo gains it, reflecting their differing electronegativities [126]. The strength of individual M – H bonds also evolve with hydrogen concentration; Ti–H bonds weaken, whereas Hf–H and Mo–H bonds strengthen, indicating element-dependent roles in absorption/desorption [126]. In TiVNb-based CCAs/HEAs, modeling and experiments suggest that local VEC affects site occupancy, with deuterium avoiding sites coordinated by higher-VEC metals [109].

4.2.2. Severe lattice distortion and strains on hydrogen uptake

Severe lattice distortion in HEAs/CCAs arises from significant atomic size mismatches among their constituent elements. This distortion creates localized tensile and compressive strain fields, leading to a highly irregular atomic structure (Fig. 16 (b)) [111]. This lattice distortion impedes dislocation movement, enhancing the strength, toughness, and deformation behavior of HEAs/CCAs. Combined with the high entropy

effect, it contributes to their superior mechanical performance compared to conventional alloys [109,110]. Severe lattice distortion creates additional interstitial sites within the lattice, where hydrogen atoms can occupy [63,109,110,141]. The occupation of hydrogen at the tetrahedral or octahedral sites induces ~20–30 % volume expansion as typical shown for the various crystal structures in Fig. 17 [112]. The occupation and increased availability of interstitial sites improves the ability of the alloy to absorb and store hydrogen efficiently [108,112,131]. Thus, the pronounced lattice distortion characteristic of CCAs/s/HEAs significantly influences hydrogen interactions [108,110]. Variations in atomic sizes and bonding properties among constituent elements lead to local deviations from ideal lattice positions, modifying the geometry and strain fields around interstitial sites [110].

Structural heterogeneity in CCAs/HEAs influences hydrogen behaviour in multiple ways. One key aspect is site availability and preference. Lattice distortion can render certain interstitial sites, which are energetically unfavourable or too small in ideal lattices, accessible to hydrogen [109,110]. For instance, in conventional BCC metals, hydrogen typically occupies tetrahedral sites; however, in distorted BCC HEAs like TiVZrNbHf, the geometry of octahedral sites (Fig. 17) can be modified sufficiently to allow substantial hydrogen occupancy [109,110]. This dual-site occupancy contributes to the higher hydrogen storage capacities observed in some HEAs compared to traditional alloys. Neutron diffraction studies have confirmed the occupation of both site types in several BCC HEA hydrides [110].

A schematic showing the hydrogen absorption mechanism and lattice evolution in BCC alloys during isothermal heat treatment is presented in Fig. 18 [142]. Initially, hydrogen diffuses into the BCC lattice, leading to gradual expansion as interstitial sites are filled. Upon saturation at elevated temperature (500 °C), the lattice reaches a stable parameter $a_{iso} > a_0$. Cooling to room temperature induces tetragonality due to hydrogen ordering, which disrupts symmetry and leads to hydrogen desorption. The lower panel compares Gibbs free energy for different interstitial sites. In the MEA TiNbZr, the tetrahedral sites are more favourable than octahedral ones [142], and their energetic stability varies with local chemistry [109,110]. Thus, the Nb-rich tetrahedral sites exhibit higher energy than Ti/Zr-rich ones, indicating preferential hydrogen occupancy in Ti/Zr-rich regions. This site-specific behavior, driven by atomic composition, governs both lattice distortion

and hydrogen retention. Overall, the emphasis is on how local atomic environments and temperature drives absorption and desorption of hydrogen behaviour in BCC metal hydrides.

Another critical factor influencing hydrogen energetics in CCAs/HEAs is binding energy modification. Local strain induced by lattice distortion directly alters the energy landscape for hydrogen accommodation [143–145]. Compressive strain increases the energy required to insert hydrogen, making absorption less favourable, whereas tensile strain reduces this energy, thereby stabilizing hydrogen at interstitial sites [21,23,143,146–149]. This strain-induced variability compounds the already broad distribution of hydrogen binding energies caused by chemical disorder in these alloys.

The electronic structure of CCAs/HEAs further modulates these energetics. The position of the Fermi level (E_F) relative to hydrogen-induced states affects hydrogen stability, while the shape and intensity of the density of states (DOS) at E_F influence the relative stability of both the metallic and hydride phases [150]. Specific electronic features, such as the d-band centre of constituent transition metals, have been shown to correlate with hydrogen binding strength and directly impact both enthalpy of solution (ΔH) and binding energy (EB) [150]. For instance, a d-band centre located deep below E_F often correlates with weak hydrogen interaction and high metal stability.

Additionally, the wide variation in local chemical environments in CCAs/HEAs produces a continuous distribution of hydrogen binding energies, which significantly affects their Pressure-Composition-Temperature (PCT) behavior. Unlike conventional hydrides that display flat pressure plateaus indicative of uniform binding energies CCAs/HEAs typically exhibit sloping plateau [109,143–145]. This slope reflects the progressive filling of interstitial sites with increasing hydrogen content, requiring higher equilibrium pressures to occupy less favourable (higher-energy) sites [112]. This energetic heterogeneity, driven by the interplay of chemical and structural disorder at the atomic level, is directly manifested in their macroscopic thermodynamic response [109].

Hydrogen diffusion is also strongly influenced by the interplay between chemical and structural disorder. The distorted potential energy landscape and variable atomic environments create irregular diffusion pathways and increase activation energy barriers for hydrogen migration [151,152]. These effects can potentially slow diffusion relative to

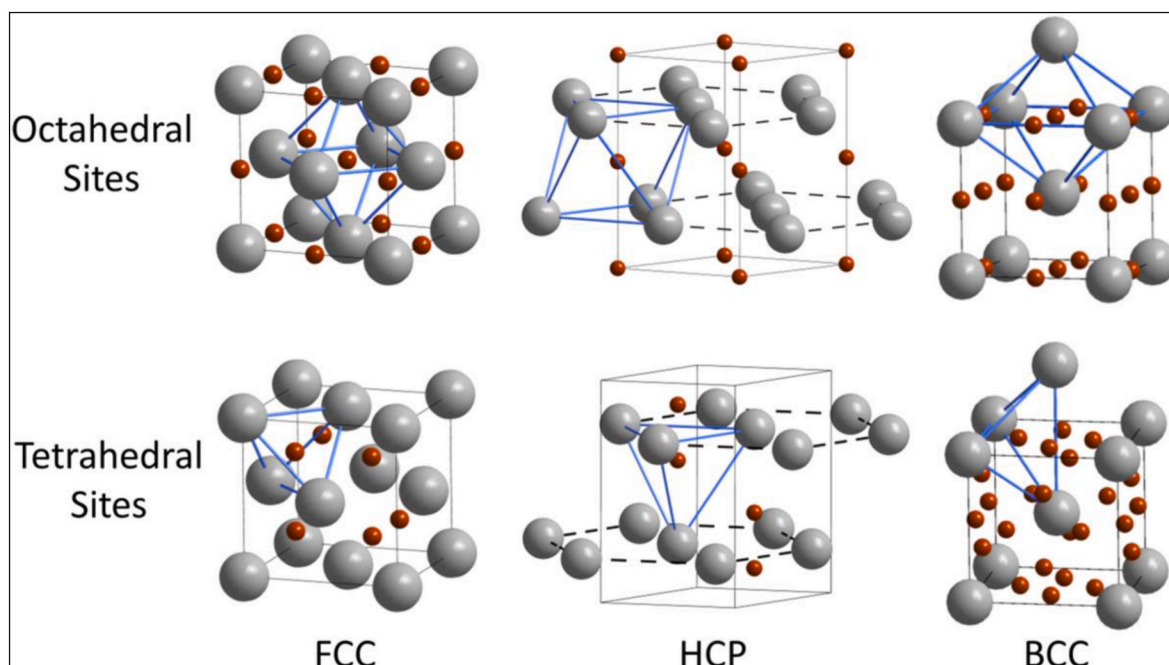


Fig. 17. Typical hydrogen occupying octahedral or tetrahedral interstitial hydride sites as indicated by brown dots [112].

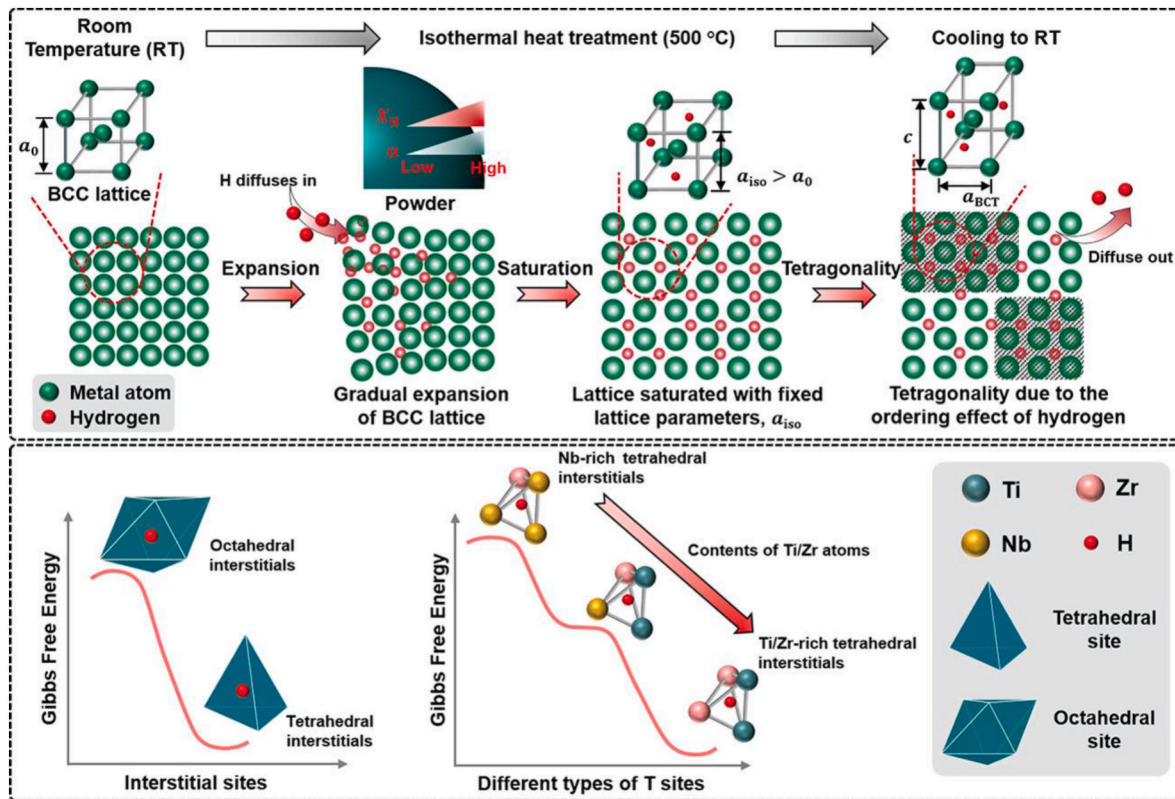


Fig. 18. Schematic of hydrogen-induced lattice evolution in BCC alloys during heat treatment, showing expansion, saturation, and tetragonality upon cooling, alongside Gibbs free energy profiles for octahedral and tetrahedral interstitial sites influenced by local Ti/Zr/Nb atomic environments [142].

that in simpler metals [152–157], although the magnitude of such changes is highly system-dependent and warrants detailed investigation.

Finally, it is essential to acknowledge that local chemical environments and lattice distortions are intrinsically linked [157]. The chemical diversity of CCAs/HEAs gives rise to lattice distortion, which in turn creates strain fields that further modify bonding interactions and site energetics [21,23,143,146–149]. As a result, fully understanding hydrogen behavior in these materials requires a holistic approach that considers chemical and structural heterogeneity simultaneously.

4.2.3. Sluggish diffusion and hydrogen uptake

The sluggish diffusion provides fundamental understandings of the kinetics effects. The HEAs/CCAs exhibit significantly slower atomic diffusion rates compared to conventional alloys, as shown in the diffusion pathways (Fig. 16 (c)). This sluggish diffusion is caused by the energy barriers created by atomic size mismatches and compositional randomness [152–154,156–158]. The slow diffusion improves the thermal stability of HEAs. Sluggish diffusion effect is associated with the formation of nano-grains within HEAs, which are typically smaller than those found in conventional alloys. These fine-grained microstructures enhance the kinetics of hydrogen absorption and desorption by shortening the diffusion paths for hydrogen atoms [159,160]. While the diffusion of hydrogen may be slower in HEAs compared to simpler materials, the presence of nano-grains can help overcome this limitation by facilitating faster hydrogen transport through the material.

Studies based on Ficks law coupled with density functional theory (DFT) were used to elucidate the kinetics and the diffusion mechanisms and pathways in HEA metal hydrides [161,162]. The modelling of the diffusion behaviours of CCAs/HEAs at the macroscopic level was done using Ficks law [26,27,43,52,163–166]. This considers the temperature and other thermodynamic conditions [154–157,167–169], whereas DFT provides critical atomic-level insights into hydrogen site preferences in

HEA-based metal hydrides [36,142,166,170–172]. This is particularly distinguishing between tetrahedral and octahedral interstitial occupancy [166,170,171], where localised lattice distortion and atomic configurations strongly influence hydrogen behaviour. This offers a predictive framework for optimizing hydrogen storage properties [36, 142,166,170–172]. Furthermore, DFT analyses guide the strategic tuning of alloy compositions to enhance hydrogen absorption and retention characteristics in high-entropy systems [36,52,142,164,166,170,171]. Sluggish diffusion is dependent on composition, crystal structure and interactions at atomic level [115,156,173–177].

4.2.4. Cocktail effects and hydrogen uptake

The cocktail effect emphasizes the synergistic contribution of all the constituent elements in HEAs/CCAs. Unlike alloys composed of a single or a few elements, HEAs exhibit complex interactions between their components that influence both their chemical and physical properties. This effect allows for fine-tuning of the hydrogen storage capabilities by adjusting the combination of elements, with each element contributing to the overall performance in terms of hydrogen absorption, storage capacity, and kinetics [66]. By carefully controlling the core effects, it is possible to engineer HEAs/CCAs with superior hydrogen storage capacities and faster absorption/desorption kinetics for next-generation hydrogen storage materials.

The cocktail effects provide the pathways for various structural and functional properties resulting from the various alloying elements. The differences in the nearest neighbour atoms and the effects on stacking sequences and fault provide exceptional underlying plasticity mechanisms. Both intrinsic and extrinsic stacking faults that contribute to their mechanical behavior through mechanisms like TRIP and TWIP [178–185]. Intrinsic stacking faults lead to localized hexagonal close-packed (HCP) stacking, enhancing transformation-induced plasticity. Similarly, extrinsic faults facilitate twinning-induced plasticity,

which improves ductility without compromising strength. These stacking faults make HEAs particularly versatile for demanding applications requiring strength and flexibility, typical for hydrogen storage.

4.3. Thermodynamic and semi-empirical parameters in HEAs/CCAs design

The design of HEA alloys is based on thermodynamic calculations and semi empirical parameters. Semi empirical parameters are derived from Hume-Rothery rules, electronegativity, valence electron concentration and atomic size mismatch are taken into consideration. The equations are used in designing and predicting solid solution formation an example of this can be seen when Yang and Zhang used Ω to evaluate the main term in Gibbs free energy (Equation (1)). They derived two scenarios one being $\Omega < 1$ enthalpy of mix is the main term and stabilises ordered phases along with intermetallic compounds while the second scenario suggests that if $\Omega > 1$ solid solution tend to form, and entropy is the main term.

$$\Omega = \frac{T_m \Delta S_{mix}}{|\Delta H_{mix}|} \quad (1)$$

where:

$$T_m = \sum_{i=1}^n C_i (T_m)_i$$

$$\Delta H_{mix} = \sum_{i < j} 4H_{ij} C_i C_j$$

$$\Delta S_{mix} = -R \sum C_i \ln C_i$$

T_m , ΔS_{mix} and ΔH_{mix} represent melting point, enthalpy of mixing and entropy of mixing respectively. These parameters are used to determine if a single-phase solid solution will form ($\Omega > 1.1$).

Atomic mismatch (δ) in HEA describes the variations in atomic sizes or arrangements among component elements, which can cause lattice distortion, phase stability influence, changes in diffusion behaviour, and changes in dislocation movement. δ is represented by Equation (2) whereby C_i is the atomic % of the i -th component, r_i is the atomic radius of the i -th component and r being the median atomic radius. Atomic size difference $\Delta\delta$ has a small value will tend to form a single-phase solid solution and a large $\Delta\delta$ will form multi-phase HEA [186]. The δ governs the possibility of CCA or HEA forming a BCC and FCC similar to valence electron concentration (VEC) as shown in Equation (3) [187,188]. The VEC plays a key role in the control of phase stability in BCC or FCC solid solutions. Authors have noted that BCC solid solutions form when the VEC < 6.87 , FCC solid solutions form when VEC > 8 while laves phase forms at a VEC of 4–8 [24,189–191].

$$\delta = \sqrt{\sum C_i \left(1 - \frac{r_i}{r}\right)^2} \times 100 \quad (2)$$

$$VEC = \sum_{i=1}^n (C_i (VEC)_i) \quad (3)$$

where n corresponds to number of components, C_i and VEC_i represent concentration and valence electron concentration of the i th component respectively.

The use of semi-empirical parameters and thermodynamic calculations via the CALPHAD approach has resulted in relatively accurate predictions of phase stability in various CCA/HEA systems. Nonetheless, the efficiency of the CALPHAD approach is heavily influenced by the quality and extent of accessible datasets [190].

4.4. Element selection and manufacturing method for hydrogen storage of HEAs

Understanding how different elements interact with hydrogen is a key component in assessing the hydrogen storage capability of an alloy. This is summarized based on the elements of the period table in Fig. 19. Enthalpy of hydride formation is central the selection of elements and the compositional design of hydrogen storage alloy. Elements can be classified as either hydride forming (A) or non-hydride forming (B) elements. The A type and B type elements are determined by the enthalpy of formation for binary hydrides which will dictate the likelihood of hydride formation. The A elements tend to form hydride phase and B elements tend to find difficulty in forming hydride phase, this is attributed to their enthalpies with elements with low enthalpies having a higher tendency to form hydride phases while elements with high enthalpies tend to struggle to form hydride phases.

The hydrogen affinity of an alloy (represented by the enthalpy of hydride formation) can be altered by mixing element with varying enthalpies. This knowledge makes HEAs an attractive storage material due to their ability to combine multiple elements while maintaining a single phase [192]. The addition of minute amounts of rare earth has also contributed to high hydrogen absorption kinetics [193–195]. For instance, Fig. 20 shows the Ce substitution and structural enhancement for hydrogen storage performance in TiFe-based alloys [193–195]. The microstructural evolution (Fig. 20 (a, b)) show how the Ce facilitates the formation of ϵ -CeH₂, which acts as an effective catalyst for hydrogen dissociation and accelerates diffusion into the TiFe matrix [194,195]. The substitution also promotes phase transitions, including the development of BCC, C14, and FCC structures, optimizing hydrogen uptake pathways [193,194]. A core-shell structure combining LaNi-based and Ti-based alloys (c) further improves hydrogen diffusion [194]. Kinetic analysis (Fig. 20 (d, e)) shows that Ce-modified alloys exhibit faster hydrogen absorption and reduced pressure decay over time compared to pure TiFe [6]. Finally, capacity measurements (f) indicate a substantial increase in hydrogen storage, from ~ 1 wt% to nearly 4 wt% post-modification. Overall, Ce alloying significantly enhances both hydrogen capacity and absorption kinetics [6,193–195].

The production of HEAs/CCAs for hydrogen storage are by various methods as summarized in Fig. 21. Generally, the production can be in the gas, liquid and solid state [21,196]. The gas state production includes molecular beam, sputtering and pulsed laser deposition. The liquid state production includes arc melting, induction melting, laser engineering net shaping and laser cladding, whereas the solid state mainly include mechanical alloying and spark plasma sintering. Based the Scopus database, most HEAs/CCAs for hydrogen storage are produced by means of Arc Melting (AM), Ball milling (BM) or Laser engineered net shaping (LENS) [21,23]. This is shown for the various classes of alloys in Table 6.

4.4.1. Arc melting (AM)

The most prominent method used for HEAs for hydrogen storage. AM is based on the principal of creating a plasma between the crucible and electrode under vacuum or inert atmosphere. The HEA is melted up to the melting point and cooled down to room temperature, this is done a few times (≥ 5) to ensure homogeneity. This is preferable for alloy production due to reduced chances of defects and the minimum chance for contamination. Possible downsides to this method would be of non-equilibrium structures which hinder a material hydrogen storage ability, this can be remedied by annealing [64].

4.4.2. Ball milling (BM)

Ball milling is a mechanical alloying method which is usually conducted in an inert or reactive atmosphere. BM is predominantly used to

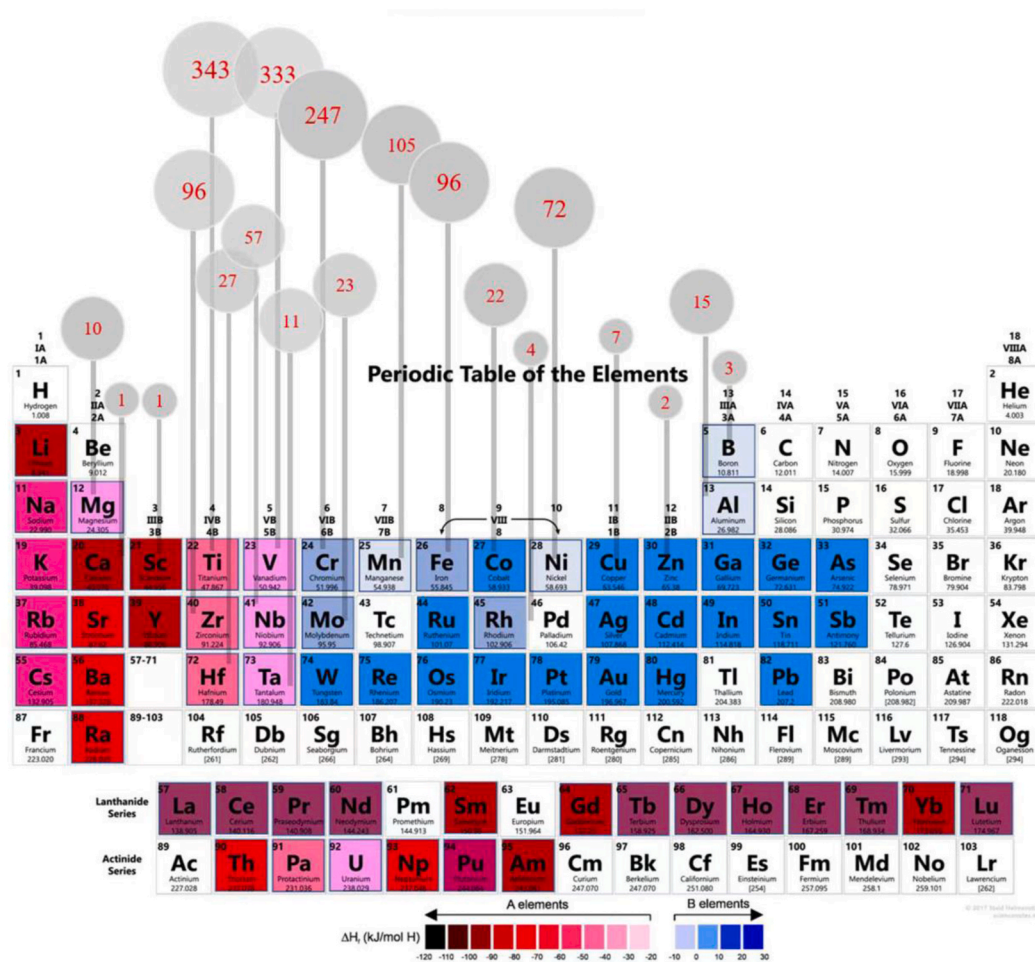


Fig. 19. Summary of various elements with varying degrees of affinity for hydrogen [21].

produce refined microstructures for equilibrium and non-equilibrium phases [263]. BM can either be conducted by mechanical alloying (MA) or reactive milling (RM) [188,267]. MA produces nanocrystalline alloys whereby repeated cold welding, fracturing and re-welding occurs under an argon atmosphere. RM is a BM method used to activate a sample for hydrogen storage by milling under hydrogen atmosphere. The particle size and alloying have controlled by the milling parameters such as rotation speed, milling time, powder to ball ratio along with the milling media [261,280].

4.4.3. Laser engineered net shaping (LENS)

LENS is a method that produces HEAs by using a laser to deposit metal powders layer by layer until a finished component is produced under argon atmosphere. This method uses a high-powered laser whereby laser power is adjusted to meet HEAs specification and melting and re-melting to ensure homogeneity. Powder size, laser power, size distribution and post processing treatment are factor that play a role in the hydrogen storage properties of HEA when using LENS [64,276]. It is important to note that this method was predominantly used Kuncze et al. in an effort to produce HEAs (TiZrNbMoV, LaNiFeVMn, ZrTiVCrFeNi) for hydrogen storage [275–277].

The first HEA based on the CoFeMnTiVZr system for hydrogen storage with a typical C14 laves phase was developed in 2010 [235]. About 1.8 wt% of hydrogen storage was observed at room temperature sparking interest in the development of HEAs for hydrogen storage due to their ability to store hydrogen at ambient conditions. When considering HEAs for hydrogen storage it is important to note the role of microstructure and activation energy, which are driven by the core effects.

4.5. HEAs/CCAs and mechanisms for hydrogen storage properties

High entropy and complex concentrated alloys combine a suite of properties that make them exceptional candidates for hydrogen storage. Their high hydrogen absorption capacity can be attributed to cocktail effects, tunable thermodynamics driven by the maximization of the configurational entropy, structural stability underpinned by the severe lattice distortions and sluggish diffusion mechanisms, and resistance to degradation and embrittlement position HEAs/CCAs as advanced materials for hydrogen storage.

Hydrogen storage capacity in metal hydrides is measured by means of weight percentage (wt %) or hydrogen to metal ratio (H/M). Hydrogen storage using HEAs is still in its infancy, with many of the mechanisms associated with HEA and hydrogen storage not understood completely. However, HEA continue to generate interest as hydrogen storage material due their ability to store hydrogen at ambient conditions compared to conventional alloys [63]. The hydrogen storage applications are attributed to the unique chemical and structural properties. These include high hydrogen absorption capacity, tailorable thermodynamic properties, excellent structural stability, resistance of HEAs to degradation, hydrogen embrittlement and cracking, great hydrogen absorption and desorption kinetics, wide and vast compositional flexibility, catalytic properties, trade-offs between volumetric and gravimetric density and environmental sustainability.

One of the most compelling features of HEAs and CCAs is their high hydrogen absorption capacity. Their multi-elemental composition creates varied atomic interactions and disordered lattice structures, which provide numerous active sites for hydrogen absorption. These features

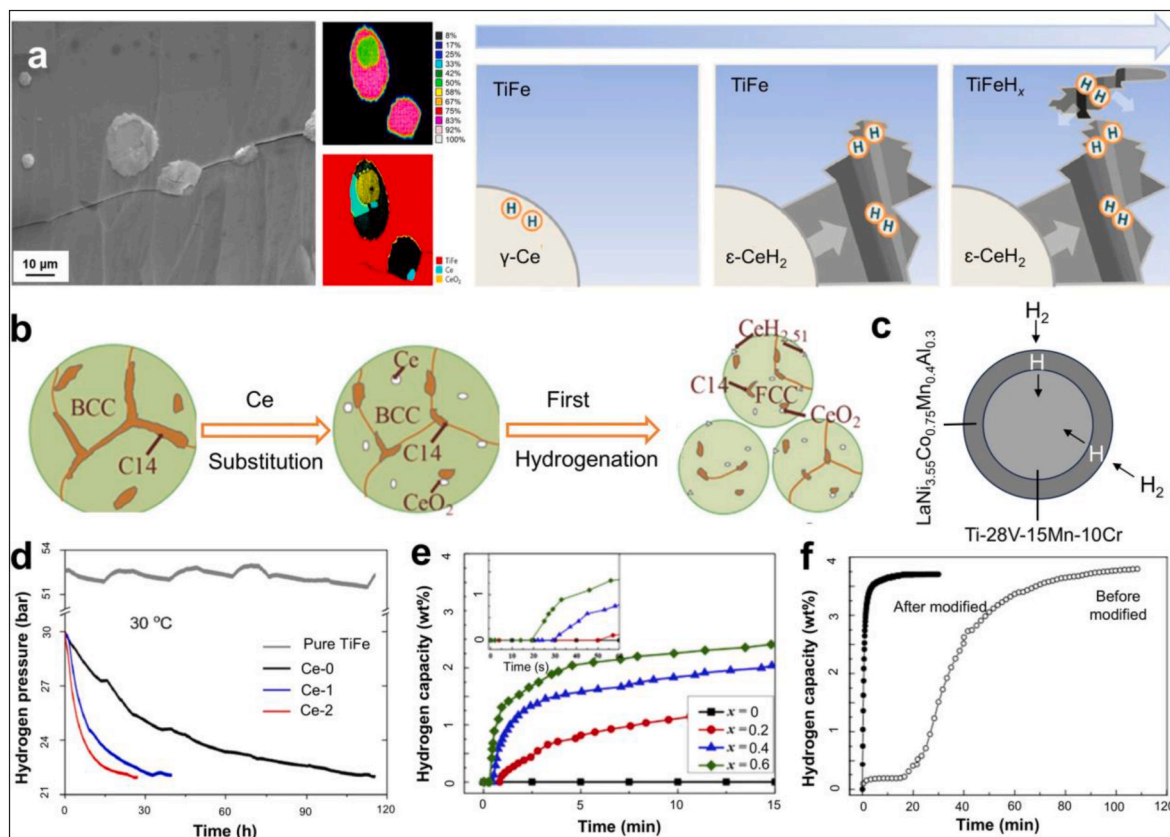


Fig. 20. Effect of minute rare earth element on hydrogen uptake with (a–c) showing microstructural evolution, phase transformation, and hydrogen diffusion mechanism in Ce-modified TiFe-based alloys [193,194]; (d–f) impact of Ce content on hydrogen pressure, absorption kinetics, and storage capacity [193–195].

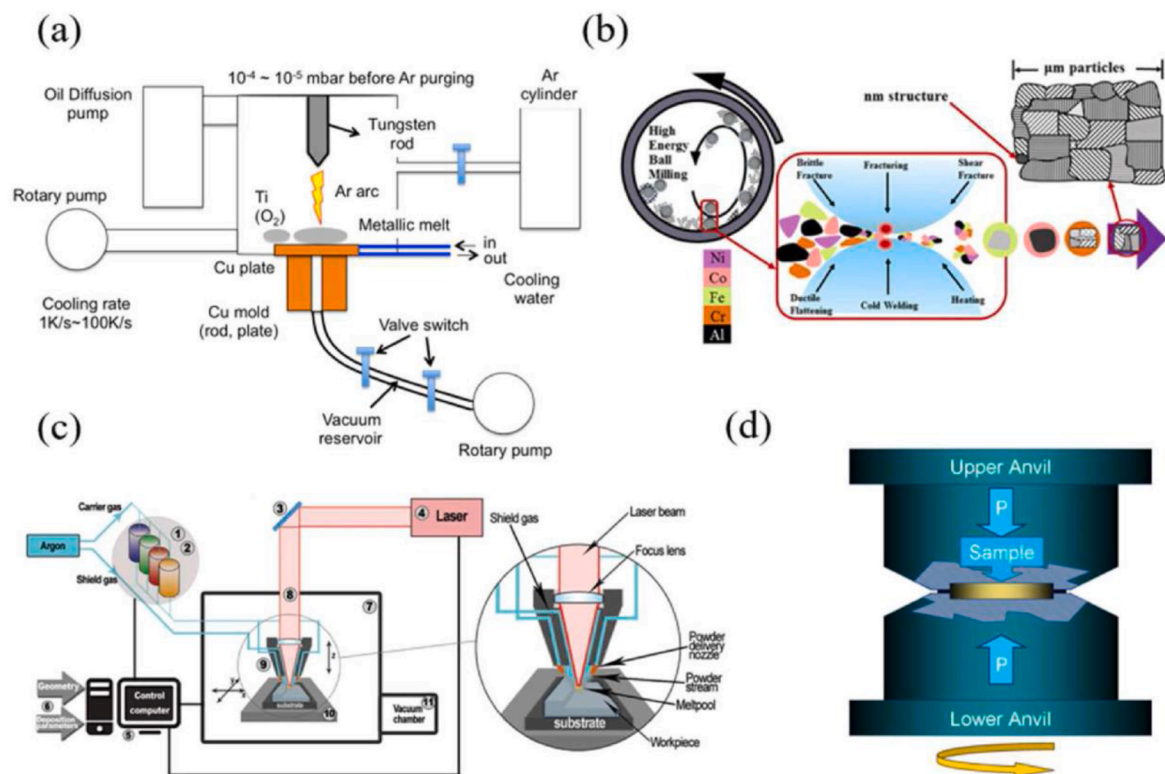


Fig. 21. Manufacturing routes of HEAs/CCAs: (a) conventional arc melting, (b) high energy ball milling for production HEA/CCA powders (c) typical LENS and (d) high pressure torsion methods [21].

Table 6

Family of HEAs, manufacturing routes and hydrogen storage properties at different temperatures.

Alloy	Synthesis method	Hydrogen storage capacity	H/M	Alloy phase	Hydride phase	Temperature	Ref
TiVNbCrFe	Arc melting/machine learning	3.25	2	BCC	FCC	Activation 683.15K for 24 and 298K	[197]
TiZrCrMnFeNi	Machine learning	1.6	–	BCC	–	303k	[198]
VNbCrMoMn		2.83	2	BCC	–		[199]
TiVZrNbHf	–	–	2	BCC	FCC	298K	[200]
Ti32.5V27.5Zr7.5Nb32.5		2,78 and 1.87	–	BCC	FCC	298k	[201]
CoCrFeMnNi	Vacuum induction gas atomiser	–	–	FCC	–	298k	[202]
NbTiVZr	Computational	2.94	–	BCC	FCC		[203]
TiZrHfMoNb		1.94	2	BCC	FCC	305K	[204]
(Ti, V, Cr, Ni, Zr, Nb, Hf, and Ta)	Arc melting	–	–	BCC	–		[205]
TiZrVMoNb		2.65	–	BCC	FCC		[206]
MgTiVZrNb		3.16	1.16	BCC	FCC		[207]
TiVNbCrNi		2.2	–	BCC	–	308k	[137]
WMoTaNbV		–	–	BCC	–		[208]
Ti-Zr-Mn-V-Fe		1.73	–	BCC	–	298k	[209]
TiVCrZrCo/TiVCrZrFe		–	–	BCC	–		[210]
TiZrFeMnCrV		1.9	–	–	–	303k	[211]
TiVZrNb		2.0	–	BCC	FCC	423k	[212]
TiVNbCrMo		2.24	–	BCC	–	323K	[213]
TiVNbMnCr		2.8	2	BCC	FCC	Activation 623k for 3 h and test at 298k	[214]
TiZrVCrNi		1.92	–	C14 Laves	–	305k	[215]
ZrCrMnFeNi		1.8	1.2	C14 Laves	–	Activated at 623k for 3 h and tested at 298k	[216]
TiZrFeMnCrV		1.92	–	C14 Laves	–	303k	[141]
TiV1.5Zr1.5CrMnFeN		1.3	0.8	C14 Laves	–	298k	[217]
TiVCrMnMoCe		3.6	–	BCC	–	Activated at 673k and tested at 358k	[218]
(Ti0.75Zr0.25)1.05Mn0.8CrTM0.2 (TM = Cr, Mo, and Nb)		1.34	–	BCC	–	Activated at 673k at test at 298k-329k	[219]
TiZrCrMnFeCoV		1.81	–	C14 Laves phase	–	303k	[192]
TiVZrNbNi		2.78	–	BCC	–	298k	[220]
TiV 2 ZrCrMnFeNi		1.6	0.92	C14 Laves	–	298k	[221]
TiZrMnFeCr		1.8	–	C14 Laves	–	298k	[222]
TiZrMnFeNi(Cr, Mo, and W)		1.6	–	C14 Laves	–	298k	[223]
TiVZrNbFe		3.19	–	C14 Laves	–	323k	[138]
TiVFeZr		2.41	1,5	C14 laves	–	Activated at 723k for 2 h and test at 293k	[224]
TiVNbZr		1.71	–	BCC	–	423k	[225]
ZrMnCrVX(Fe, Co, Ni and Cu)		1.4	–	C14 laves	–	373k	[226]
TiVNbCr		–	1,9	BCC	FCC	Activation at 723k for 4 h and testing at293k	[227]
TiZrVNBa		1.8	1,7	BCC	–	293k	[228]
TiZrHfTa		–	–	BCC	HCP		[229]
Ti4v3NbCr2		3.7	2	BCC	–	300k	[230]
TiZrMnCrFeCu		1.8	–	C14 laves	–	Activation 473k and tested 298k	[231]
TiVZrNbFe		1.6	–	C14 laves	FCC	298K	[232]
TiZrNbCrFeNi		1.5	–	C14 laves	–	298k	[233]
TiVNbCr		3.7	–	BCC	–	300k	[234]
CoFeMnTiVZr		1.8	–	C14 laves	–	298k	[235]
TiVMnZrNb		2.98	2	BCC	FCC	298K	[236]
TiZrNb, TiZrNbHf and TiZrNbHfTa		–	–	BCC	FCC		[237]
TiNbFeMnCr		1.4	–	C14 laves	–	298k	[238]
TiVZrNb(Mg, Al, Cr, Mn, Fe, Co, Ni, Cu, Zn, Mo, Ta)		–	2	BCC	FCC	298k	[239]
TiZrCrMnFeNi		1.6	1	C14 Laves	–	298K	[240]
VTiCrMnNb		3.45	–	BCC	FCC	298K	[241]
TiZrVCrNi		1.52	–	C14 laves	–	298K	[242]
TiVCrZrNb		3.0	2	BCC	FCC	298K	[243]
TiZrFeMnCrV		1.8	–	C14 laves	–	303k	[63]
ZrTiVAlFe		1.58	–	C14 laves	HCP	473k	[244]
TiZrHfMoNb		1.75	1.8	BCC	FCC	523k	[245]
ZrTiNiCrMn		1.66	–	C14 laves	–	323k	[246]
(ZrTiVFe)Al		1.3	–	C14 laves	HCP	298k	[247]
TiVZrNbMo		2.8	2	BCC	FCC	298k	[248]
TiZrNbCrFe		1.8	1.32	C14 laves	–	473k	[249]
TiVNb (Cr, Ni or Co)		3.2	2	BCC	FCC	473k	[250]
TiVNbX (Cr, Mn, Fe, Co, and Ni)		–	2	BCC	FCC	298K	[251]
TiZrHfNb		–	1,5	BCC	FCC	573k	[252]
TiVZrNbH		–	2	BCC	FCC	613k	[253]

(continued on next page)

Table 6 (continued)

Alloy	Synthesis method	Hydrogen storage capacity	H/M	Alloy phase	Hydride phase	Temperature	Ref
TiZrNbFeNi	Ball milling	1.64	–	C14 laves	–	305k	[254]
TiZrHfMoNb		1.54	–	BCC	FCC	873k	[255]
TiVZrNbTa		2.5	2	BCC	FCC	298k	[256]
TiZrCrMnFeNi		1.7	1	C14 laves phase	–	298K	[257]
TiZrNbTa		1.67	–	BCC	–	293k	[258]
TiVNbTa		2.66	–	BCC	FCC	493k	[259]
TiVNbX(Cr,Zr,Mo,Hf)		1.96	2	BCC	FCC	298k	[260]
TiZrNbHfTa		–	2,5	BCC	FCC	298k	[70]
TiVFeCuNb		0.6	–	BCC	–	473k	[261]
ZrTiVFe		0.37	–	C14 laves	–	673k	[262]
VTiCrFeMn		0.36	–	BCC	–	623k	[263]
Mg ₈ (TiVCrNb) _{100-x}		2.93	1.62	BCC	FCC	298k	[264]
FeCoNiCrTi		–	–	–	–	–	[265]
AlMg2TiZn		1.4	–	BCC	–	643k	[266]
MgAlTiVZn		2.5	–	BCC	FCC	648k	[267]
MgTiVZrNb		2.7	1,7	BCC	–	298K	[268]
MgVAlCrNi		0.3	–	BCC	–	655k	[269]
AlCrFeMnNiW		0.62	–	BCC	FCC	298k	[270]
MgTiVCrFe		0.9	–	BCC	–	623k	[271]
MgZrTiFeCoNi		1.2	–	BCC	FCC	623k	[272]
MgAlTi(X)Ni		2.1	–	BCC	B2 ordered	473k	[273]
MgAlTiFeNi	Mechanical alloying and Reactive milling	0.94	–	BCC	FCC	373k	[274]
LaNiFeVMn	LENS	0.83	–	sigma phase	FCC	308k	[275]
TiZrNbMoV	Induction melting	2.3	–	BCC	–	298k	[276]
ZrTiVCrFeNi		1.81	–	C14 laves	–	Activated at 773k for 5 h and tested at 323k	[277]
LaMgNiCoCu		–	1,6	BCC	–	298k	[278]
LaCePrNdNi		1.3	–	–	–	303k	[279]
CoMnAlCuZrFe		–	–	–	–	–	–

facilitate the formation of stable hydride phases, a critical requirement for achieving efficient hydrogen storage. The kinetics of hydrogen absorption and desorption are superior in HEAs and CCAs due to their multiple catalytic sites [21,23,31,33,71]. The synergistic effects of various alloying elements improve diffusion pathways and reduce activation barriers, enabling fast and more efficient hydrogen storage and release. This property is vital for applications requiring rapid hydrogen cycling. The catalytic properties of HEAs and CCAs also play a significant role in their hydrogen storage capabilities. These materials facilitate the dissociation and recombination of hydrogen molecules, reducing the energy required for absorption and release [40,44,71,281,282]. This enhances their efficiency and makes them more economically viable for hydrogen storage applications.

A significant advantage of HEAs and CCAs lies in their tailorable thermodynamic properties. The compositional flexibility of these materials enables precise control over their thermodynamic behavior, allowing for optimization of hydrogen absorption and desorption temperatures and pressures. The compositional flexibility of HEAs and CCAs further enhances their appeal [13,21,31,33,71]. These materials can incorporate elements like titanium (Ti), vanadium (V), zirconium (Zr), magnesium (Mg), and nickel (Ni), known for improving hydrogen storage properties. This flexibility allows for the design of alloys tailored to meet specific requirements, such as high storage capacity, low cost, or compatibility with operational conditions [13,21,31,33,40,44,71,281,282]. This adaptability enhances their practicality for real-world hydrogen storage and release conditions. Generally, HEAs and CCAs exhibit remarkable structural stability under extreme hydrogenation and dehydrogenation cycles. Their typical single-phase solid solution microstructures, such as body-centered cubic (BCC) or face-centered cubic (FCC) forms, prevent phase separation and structural degradation. This ensures the longevity and reliability of the materials, even under demanding operational conditions.

Unlike conventional materials, HEAs and CCAs demonstrate

exceptional resistance to hydrogen embrittlement. This is attributed to their high configurational entropy, which disrupts localized stress concentrations and minimizes crack propagation. Such resilience makes these alloys durable under prolonged hydrogen exposure, addressing a critical challenge in hydrogen storage materials. In addition to their superior mechanical properties, HEAs and CCAs are inherently resistant to degradation. They demonstrate exceptional resistance to oxidation, corrosion, and other forms of wear, ensuring longer operational life. This robustness makes them suitable for repeated use and operation in harsh environments.

The HEAs and CCAs achieve favourable balance between volumetric and gravimetric hydrogen densities. This balance is crucial for applications where lightweight design and high storage capacity are essential, such as in portable or transportation-related hydrogen systems. These alloys provide practical solutions for achieving optimal performance under such constraints. Most HEAs and CCAs align with environmental and economic sustainability goals. They can be designed using earth-abundant and inexpensive elements, reducing dependence on costly and rare materials. This feature enhances their economic feasibility while maintaining excellent performance in hydrogen storage applications.

4.5.1. Microstructural effects on hydrogen storage properties

Single phase HEAs for hydrogen storage perform better than conventional alloys at ambient conditions. Amongst these HEAs, the BCC types show better hydrogen storage capabilities than other HEA alloys [251]. Generally, BCC HEA average an H/M of 2 which is considerably high compared to other HEAs with different phases. The availability of vacancies in BCC structures make them desirable hydrogen occupation during storage [251,283]. The BCC phase forms when VEC < 6.87, which can be calculated by CALPHAD [24,189–191]. It is important to calculate enthalpy and entropy of the alloy along with the atomic mismatch to ensure BCC single phase can be formed. However, BCC alloys do have

poor kinetics and poor hydrogen reversibility. Similarly, these alloys also have poor absorption and desorption properties while boosting great hydrogen storage capability at mild conditions [283].

The microstructural feature of critical importance to hydrogen storage capacity in CCAs/HEAs metal hydrides is the formation of Laves phases. These intermetallic compounds, classified into three main crystal structures which are C14, C15, and C36 can accommodate significant amounts of hydrogen [220,244,284]. Their crystalline frameworks enable efficient storage through a combination of physisorption and chemisorption mechanisms [284]. The specific composition and structural arrangement of HEAs affect the interaction dynamics between hydrogen and the alloy, influencing both capacity and kinetics [220, 244]. The stability of Laves phase-containing HEAs under varying pressure and temperature conditions further enhances their suitability for hydrogen storage applications [220].

Laves phases have gained considerable attention due to their ability to reversibly absorb substantial hydrogen quantities. Under moderate operational conditions, minimal or no activation energy is required to induce the absorption process [238]. Furthermore, alloys with Laves phases can store hydrogen in the presence of air without thermal activation [285]. The Laves phase typically serves as the initial site for hydrogen absorption, contributing to the observed improvements in hydrogen storage kinetics [286]. Alloying elements such as Fe, Ti, Zr, and Ni promote the formation of C14-type Laves phases, enhancing both storage capacity and kinetic performance [286]. Although Laves phases generally store around ~ 1 H/M, which is lower than the ~ 2 H/M typically achievable in BCC structures, their main advantage is superior hydrogen absorption and desorption kinetics, making them highly attractive for practical hydrogen storage systems [287].

A TiZrNbCrFe HEA was synthesized, predominantly consisting of a C14 Laves phase with a minor BCC phase fraction. The alloy had superior hydrogen absorption capabilities compared to conventional C14-type alloys, with a hydrogen-to-metal ratio (H/M) of 1.32 [249]. This was relatively higher than the typical 1 H/M observed in standard C14 alloys [287]. The maximum hydrogen absorption was recorded at 1.9 wt % at 200 °C [249]. Similarly, a $\text{Ti}_{0.24}\text{V}_{0.17}\text{Zr}_{0.17}\text{Mn}_{0.17}\text{Co}_{0.17}\text{Fe}_{0.08}$ alloy was synthesized using Thermo-Calc simulations with ~ 98 % C14 Laves phase content [288]. Although the Laves phase demonstrated lower overall storage capacity compared to BCC phases, it showed significantly faster absorption and desorption kinetics. The alloy achieved a maximum storage capacity of 0.72 wt%, lower than the 1.91 wt% typically expected for C14 phases [249]. However, it was able to absorb 0.53 wt% hydrogen within ~ 15 s, highlighting its excellent kinetic performance [288].

There is the need for dual phase to optimize hydrogen storage capacity and kinetics in HEA-based metal hydrides. This is the case for CCAs/HEAs with Laves phases and BCC matrix structure. Thus, a predominantly BCC structure provides sufficient hydrogen storage capacity [251,283], whereas the Laves phases promote hydrogen absorption and desorption kinetics [220,244,284]. Together, these structural features significantly improve the practicality and performance of HEA metal hydrides, making them more viable candidates for applications within

the evolving hydrogen economy.

4.5.2. Activation mechanisms

The first hydrogenation tends to be slow and the need for high pressures and temperatures are required to assist the process. This is known as activation, which employs varying temperatures with different holding durations to stimulate hydrogen atoms, thereby augmenting their kinetic energy [209]. However, this often has a detrimental effect on the storage capacity [289], particularly evident in TiVZrHfNb alloys where increased activation temperatures lead to faster hydrogen absorption but at the cost of reduced storage capacity.

The activation mechanisms for efficient hydrogen absorption and desorption can be understood based on the exceptional structural and compositional properties of the materials. Fig. 22 shows the schematic of the activation mechanisms associated with CCA/HEA metal hydride formation [37,45,151,290–292]. Key mechanisms include the role of interphase boundaries in facilitating hydrogen transport and nucleation [151]. Dual-phase HEAs/CCAs, exemplified by TiVZrCrMnFeNi, exhibit enhanced hydrogen absorption kinetics at room temperature compared to their single-phase counterparts [38,45,151,290,293,294]. The dual phase lowers the energy barrier for hydrogen absorption and desorption and is shown in TiZrCrMnNi (VFe) [13,31,33,45,151]. The interphase boundaries in most BCC HEAs are pathways for hydrogen diffusion and catalyze hydride formation, eliminating the need for high-temperature activation [38,290,293,294]. Another mechanism is the use of high-pressure torsion processes to produce favourable lattice defects that enhance hydrogen kinetics [291]. This serves as nucleation sites for hydrogen absorption. This method significantly improves the activation of HEAs, allowing for absorption of hydrogen rapidly even after prolonged air exposure [29,35,42,49,59,291,293–299]. Furthermore, valence electron concentration can be optimized to stabilize hydride formation [33,292]. For instance, an alloy with a VEC of 6.4 and a single-phase C14 Laves structure, such as TiZrCrMnFeNi [33,292], can absorb and desorb hydrogen efficiently at room temperature without activation treatment [151,294,297]. Additionally, elemental doping plays a critical role by destabilizing surface oxides, thereby optimizing electron density and reducing interfacial energy [31,33,290]. Activation mechanisms that reduce surface oxides to suboxides and sub-hydroxides can significantly enhance hydrogen absorption kinetics. This is observed in TiZrNbTa HEAs, where activation reduces oxides, facilitating hydrogen uptake at lower temperatures [31,33,290]. The high zirconium (Zr) content promotes the formation of stable intermetallic phases, further enhancing the activation mechanisms necessary for effective hydrogen storage [151,291,292].

Hydrogen storage properties was achieved in $(\text{TiVNb})_{0.90}\text{Cr}_{0.05}\text{Mn}_{0.05}$ at 623K for 3 h and tested at 298K [214]. An improvement in hydrogen storage kinetics at room temperature with increasing activation temperature was observed. However, there are drawbacks associated with first hydrogenation activation. This is because not all hydrogen storage HEAs undergo activation and simultaneously have good hydrogen storage kinetics. Thus, there is the need for understand the thermodynamic and kinetic principles driving the

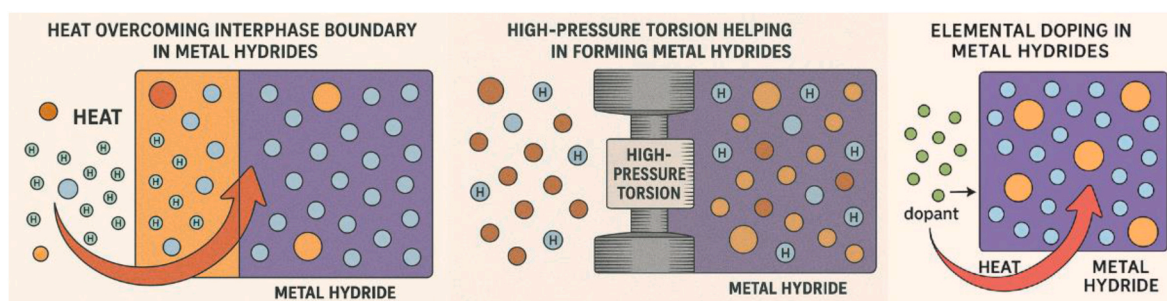


Fig. 22. Schematics showing activation mechanisms in CCA/HEA metal hydride.

mechanisms responsible for hydrogen storage properties. Table 6 shows an overview of various HEAs and their hydrogen storage properties. A notable trend is the prevalence of the BCC (Body-Centered Cubic) crystal structure among these alloys, suggesting its favourability for hydrogen storage applications in this class of materials. While the hydrogen storage capacities vary, several alloys demonstrate promising values exceeding 2 wt%, indicating the potential of HEAs as viable hydrogen storage media.

Synthesis methods employed include arc melting and machine learning, highlighting the growing role of computational approaches in designing novel HEAs with enhanced properties. The presence of certain elements, such as Ti, V, Zr, Nb, and Cr, appears to be common in alloys exhibiting higher hydrogen storage capacities [13,31,33,45,151]. This lends credence to the BCC type CCAs/HEAs being the favourable constituent elements with good hydrogen storage capabilities.

While valuable insights are provided, further investigation is necessary. For instance, the correlation between the C14 Laves phase and specific hydrogen storage behaviors requires further exploration. Additionally, a more comprehensive analysis of the H/M ratio (hydrogen atoms per metal atom) is needed to determine its influence on hydrogen storage capacity.

4.5.3. Degradation mechanisms

Metal hydrides can absorb large amounts of hydrogen, however over time the hydrogen performances of these materials suffer due to different degradation mechanisms. HEA metal hydrides gradually show a decline in hydrogen storage performance over several hydrogen absorption and desorption cycles which lead to the degradation of HEA metal hydride [300].

Degradation in HEA metal hydrides can be caused by mechanical stress induced by repeated absorption and desorption during hydrogen cycling which will result in the contraction and expansion of the crystal lattice [301]. The entering and existing of hydrogen atoms in the metal lattice causes volume changes to contribute to dislocations formations along with microcracks and pulverization of HEA particles [302]. This results in a reduction in structural integrity along with hydrogen storage performance of the metal hydrides.

Phase segregation during hydrogenations can be a contributing factor in degradation of HEA metal hydrides. HEAs developed and designed for phase stability, the addition of hydrogen atoms leads to a disturbance in the distribution of atoms which results in secondary phases or elemental segregation [204]. Phase segregation due to hydrogenation results in reduction in uniformity of the alloy which will cause areas of inactivity for hydrogen storage. The reversibility of metal hydrides can be decreased in some cases whereby a stable hydride phase is formed but does not release hydrogen efficiently [303].

HEAs with elements such as Ti, Cr or Al have a likelihood of surface oxidation. A HEA metal hydride that is exposed to air or moisture can lead to the creation of an oxide layer on the surface of the metal particles. The oxide layer can act as a barrier to hydrogen atom and hydrogen diffusion thus resulting in the reduction of kinetics during hydrogen absorption and hydrogen desorption [304,305]. Surface oxidation can additionally cause structural changes such as grain coarsening over a period of time especially at high temperatures, this can reduce the surface area and hinder hydrogen transportation [306].

These degradation mechanisms have spurred a lot of research interest which has led to the exploration of several strategies. One approach to combating degradation of HEA metal hydrides would be optimizing of the alloy composition with the aim of avoiding elements that form stable and impermeable oxides [307]. Protective coatings like thin titanium dioxide, can assist in controlling oxidation while providing a pathway for hydrogen to pass through [308]. Hydrogen storage kinetics can be improved by nanostructuring and ball milling by means of uniform microstructures with shorter diffusion paths [309]. Operating under mild hydrogenation conditions can reduce the mechanical stress while extending cycling life of HEA metal hydrides.

5. Computational material design

Computational modelling is often used in order to reduce cost and eliminate the need for trial and error by developing a model that satisfies required properties prior to actual testing, thus limiting cost and material. The recent computational approach uses machine learning (ML) to design, optimize and predict composition, structures and properties of materials. A typical workflow and process for the application of machine learning in material science is given in Fig. 23 [3]. The basic ML workflow typical for the design and discovery of materials show a closed-loop framework from data preparation to model deployment. The process commences with dataset establishment, including preprocessing, splitting into training, testing, and validation sets [3,61,310–316]. Next, feature engineering involves down-selection and dimensionality reduction to refine inputs. These features are used in model training, applying algorithms such as regression or classification (e.g., KNN, RF, SVM, GBDT, CNN, GNN) [3,61,310,317–319]. After training, model performance is validated through experiments or simulations, enabling model re-optimization. This iterative loop supports property prediction, space exploration, and inverse design. Ultimately, the framework promotes continuous improvement and generalization, enhancing material discovery and performance prediction across diverse systems [318].

A Sankey diagram comprising of complex network visualization focusing on the relationships between various ML models and their applications in different materials science domains is given in Fig. 24 [317]. This is densely interconnected, suggesting a rich interplay between different ML algorithms and their analysis in predicting various material properties. The prominent ML models include Support Vector Machines (SVM), Random Forests and Neural Networks (NN). These models are connected to various dilute and compositionally complex alloys.

The thickness and colour of the connecting lines likely represent the frequency or strength of the relationship between a particular ML model and a material category. This network visualization provides a valuable overview of the current state of ML applications in materials science, highlighting the diverse set of tools available for researchers and the growing interconnectivity between different fields within this domain. Among the most promising techniques, Support Vector Regression (SVR) has proven effective in predicting the hydrogen-to-metal ratio (H/M) and valence electron configuration (VEC) in HEAs [320]. Its strength lies in handling complex relationships between variables. Similarly, K-Nearest Neighbours (KNN) has been applied to predict HEA properties [320], particularly in combination with other algorithms. This simple yet effective technique is well-suited for small datasets.

Random Forest (RF) has gained recognition for predicting key hydrogen storage properties, including heat of formation, phase abundance, and hydrogen capacity [320,321]. Its accuracy and robustness make it ideal for handling large datasets. Gaussian Process Regression (GPR) is another promising method [322], providing predictions for hydride formation enthalpy while also offering uncertainty estimates. Gradient Boosting Regression (GBR) has shown high accuracy in predicting catalytic activity and other HEA properties [323], making it invaluable for managing complex datasets. Furthermore, Artificial Neural Networks (ANN) stand out for their capability to model highly non-linear relationships [324,325], often applied to predict mechanical properties and phase formation. Decision Trees and ensemble methods such as Extra Trees, AdaBoost, and Bagging enhance accuracy and provide interpretable models [324], particularly in predicting phase formation and mechanical properties.

Key applications of ML in hydrogen storage include predicting hydride thermodynamics and capacities, which enable rapid screening of HEAs with desirable storage characteristics [326]. Techniques like RF and ANN are particularly effective for phase prediction and mechanical property analysis, critical for designing HEAs with optimal hydrogen absorption and desorption capabilities [320,321,324,325]. ML also facilitates the optimization of alloy compositions, reducing reliance on

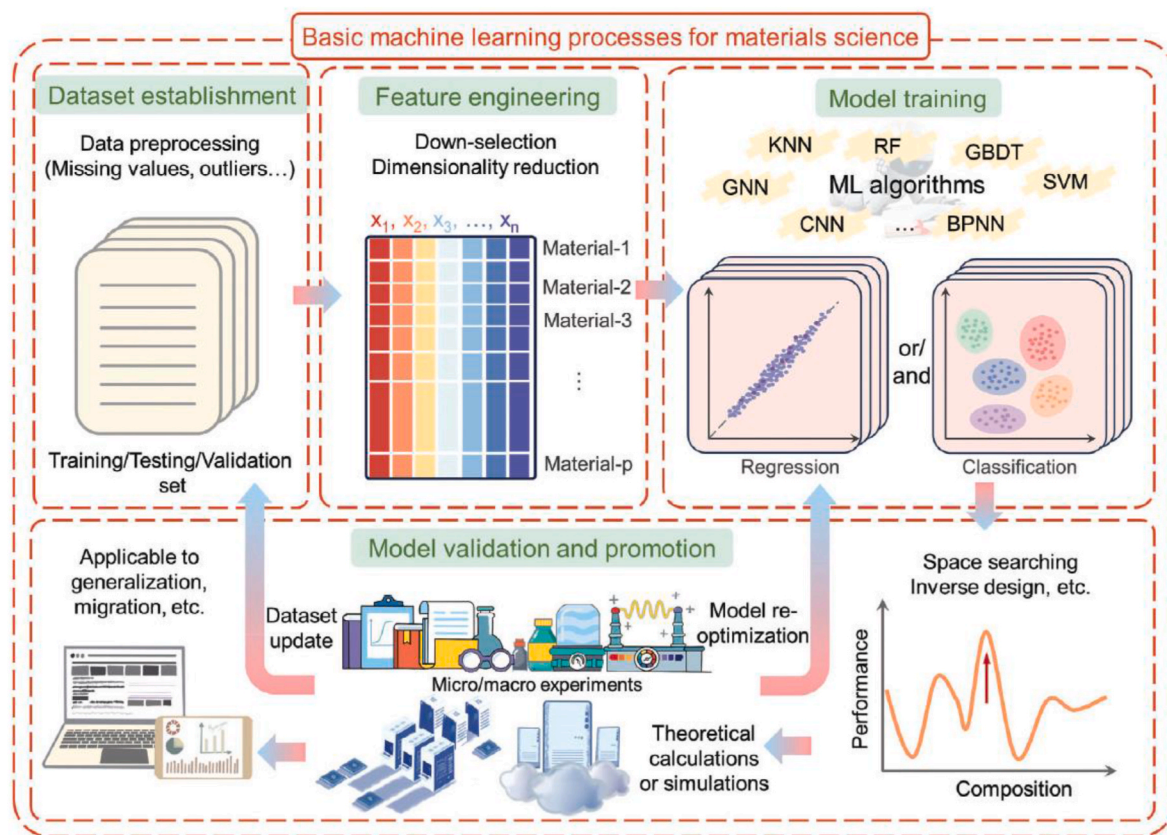


Fig. 23. Typical machine learning procedure and workflow in materials discovery showing the closed-loop framework [3].

labour-intensive experimental trials. High-throughput screening powered by ML enables the evaluation of thousands of HEA compositions, identifying the most promising candidates for hydrogen storage [39, 323–327]. Thus, integrating ML techniques such as SVR, KNN, RF, GPR, GBR, ANN, and ensemble methods has significantly advanced the study of hydrogen storage in HEAs. These approaches enhance prediction accuracy, accelerate alloy discovery, and optimize material performance, making ML an indispensable tool in hydrogen storage research. By combining computational insights with experimental validation, ML is poised to revolutionize the development of sustainable energy solutions.

First principle computational material design tools have been used to predict the hydrogen storage capability of HEA. One of the initial studies was the modelling of TiZrHfMoNb alloy for hydrogen storage [204]. A hydrogen storage capacity 1.94 wt% and H/M of 2 was predicted using the density functional theory (DFT). Furthermore, TiZrVMoNb HEA was developed for hydrogen storage by means of computational modelling predicted a BCC HEA with a hydrogen storage capacity of 2.65 wt% [206]. Computational modelling assisted in predicting the phase transformation (BCC- FCC), analysing site preferences, predicting maximum hydrogen storage capacity and assist in comparing hydrogen storage properties of different HEAs. This HEA was modelled by using DFT which helped understand the hydrogen interactions and phase stability within HEAs [206]. A density functional theory based on Vienna Ab initio Simulation Program (VASP) was used to designed NbTiVZr alloy to predict hydrogen storage capacity of 2.94 wt% and the transformation from BCC to FCC [203]. Thus, NbTiVZr was selected for its superior mechanical properties, showing increased bulk, shear, and Young's moduli with hydrogen uptake indicating greater stiffness and deformation resistance [203]. The use of VASP significantly reduced the time and cost of evaluating hydrogen storage properties in the metal hydride. As a first-principles tool, it effectively simulates hydrogen

behaviour, although limitations include neglecting van der Waals interactions and oversimplifying material deformation under stress, which may not capture real-world complexity [204,206,207]. This can be addressed by incorporating metal-hydrogen interactions, refining simulation parameters, and leveraging physics-based machine learning models.

Hydrogen storage capacities in HEAs are predicted by ML and achieved promising results such as 3.25, 1.6, and 2.83 wt% [328,329]. These studies demonstrate that ML can significantly accelerate the discovery of suitable HEA compositions for hydrogen storage, offering a cost-effective alternative to traditional trial-and-error methods [328–330]. ML excels at handling the complex, high-dimensional, and non-linear relationships between composition, structure, and properties, enabling tailored customization of HEAs to meet specific hydrogen storage requirements [197–199]. Table 7 summarizes recent advancements in applying machine learning (ML) techniques to predict hydride-related properties in HEAs and CCAs. It showcases a range of ML models including supervised learning [331], ensemble methods [312], regression trees [322,332], and neural networks [333] used to predict key thermodynamic parameters such as enthalpy of formation (ΔH), hydrogen-to-metal ratios, sorption capacity, and hydrogen storage capacity. These studies span diverse alloy systems, including BCC, AB₂-type, and multicomponent high-entropy alloys. Notably, several approaches integrated ML with DFT data to enhance predictive accuracy and identify promising hydride-forming compositions. Large databases, such as ML-HydPARK and datasets from the US Department of Energy, were frequently employed to train and validate models [334–338]. Importantly, ML techniques have facilitated high-throughput screening, structure-property relationship discovery, and the rational design of hydrogen storage materials with improved performance, accelerating experimental efforts in the field (Table 8). The evaluation metrics for evaluating the error functions based on the various ML models with

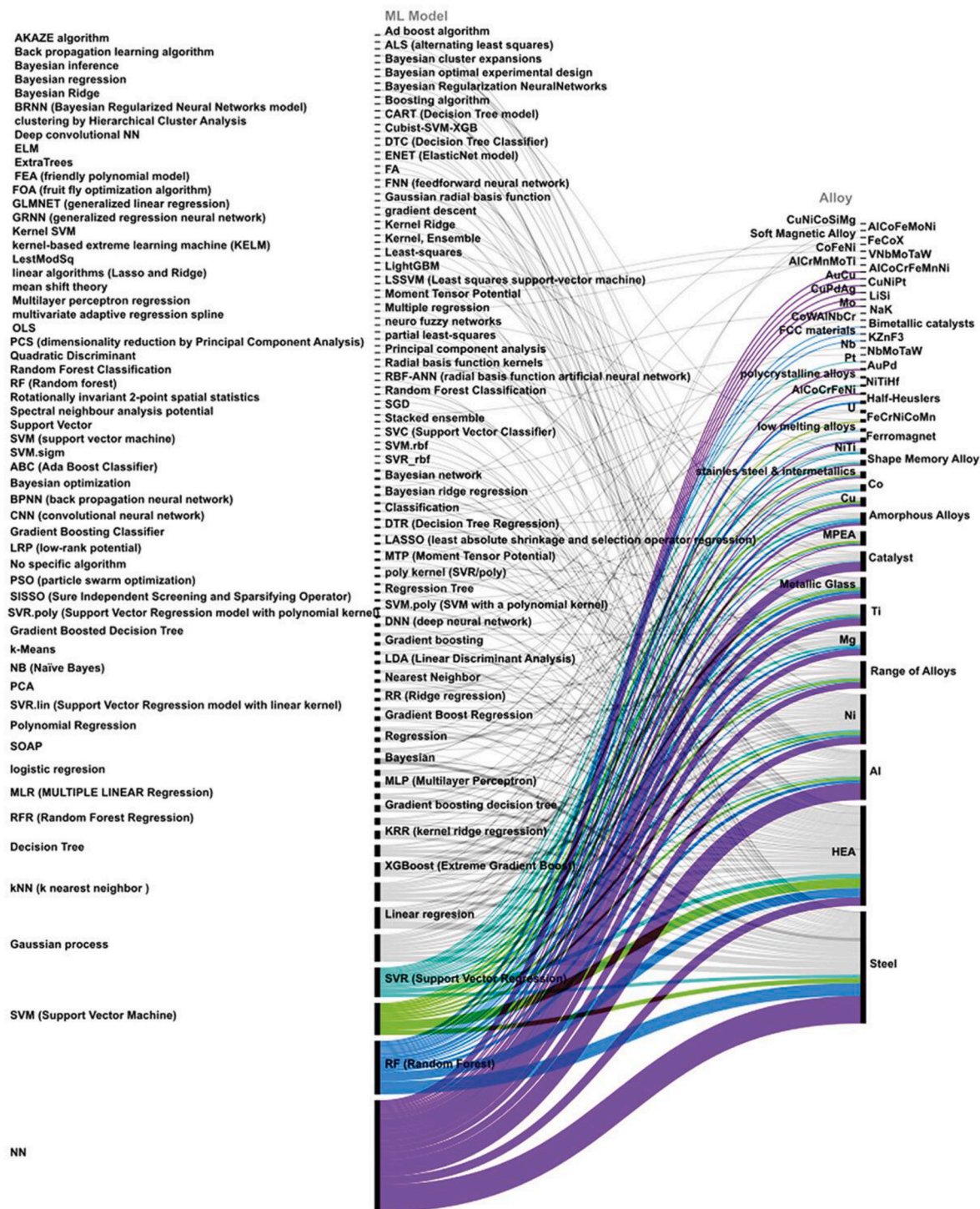


Fig. 24. Network visualization depicting the relationships between various machine learning algorithms and their applications in different materials science domains [317].

relevant equations are given in Table 9 [3]. Furthermore, some of the latest databases for traditional and physics-based machine learning based prediction of CCA/HEA hydrides are summarized in Table 10.

There have been discrepancies between predicted and experimental hydrogen storage capacities. These inaccuracies are attributed to the complex atomic arrangements within the alloys [197–199]. Machine learning models heavily rely on data, necessitating large volumes of high-quality data for accurate predictions [312,318,319,332,333, 338–340,369]. Furthermore, the intricate relationships between

composition, structure, and hydrogen storage capacity pose significant challenges for precise predictions. Additionally, models trained on specific datasets may struggle to generalize to new or unseen compositions [370], especially those involving elements not included in the original training data. Addressing these challenges is crucial for improving the reliability of machine learning in HEA design for hydrogen storage. As more research on HEA hydrogen storage is conducted, the availability of data will increase, leading to improved ML models for this application [197–199].

Table 7

The CCAs/HEAs metal hydrides predicted using ML.

HEA/CCA composition(s)	Machine learning technique(s)	Predicted property (related to hydride formation)	Notes	Reference
HfMoNbTiZr	Supervised Machine Learning (integrated with DFT-SQS)	Enthalpy of hydride formation (ΔH_f) for MH and MH ₂	Explore a large chemical space of quinary BCC HEAs for hydrogen storage	[331]
HfNbTiVZr			High-throughput computational screening study guided by ML	
HfNbTaTiZr			Hydrogen storage material using a combination of DFT and ML	
MoNbTiVZr			Quinary BCC HEA composition studied within the ML-accelerated framework	
Various Low-, Medium-, and High-Entropy Alloys (including BCC, C14, and C15 structures)	Linear Regression	Hydrogen storage capacity (sorption capacity, thermodynamics, enthalpy of hydride formation)	Analysis of large dataset (>350 entries) to identify correlations and enable predictions across different multi-component alloys.	[339]
Various Metal Hydride Compositions (from ML-HydPARK database, >1200 entries)	Interpretable Machine Learning, Gradient Boosting Tree Regressors/Classifiers (various algorithms utilized with the dataset)	Enthalpy and entropy of hydriding reaction, Maximum hydrogen capacity, Hydride stability	ML models trained on a curated database to predict key thermodynamic properties and hydrogen storage capacity.	[322, 332]
Ti _x Zr _{2-x} CrMnFeNi (x = 0.5, 1.0, 1.5) (AB ₂ -type HEAs)	Gaussian Process Regression (GPR) with various kernels, Multivariate Regression, Support Vector Machine, Regression Tree	Enthalpy of hydride formation	ML predictions were validated against experimental and DFT data for designing HEAs for targeted room-temperature hydrogen storage.	[322]
Ti-Nb-X ternary alloys (where X = Mo, Cr, Hf, Ta, V, Zr)	Random Forest, Extreme Gradient Boost, Gradient Boost	Hydrogen-to-Metal (H/M) ratio, Solution Energy, Hydrogen weight percent	Explored compositional effects within ternary HEA families on hydrogen storage using ML-guided approach.	[333]
Co-Ni-X ternary alloys (where X = Al, Mg, V)			Hydrogen storage potential of different ternary alloy systems using ML to predict key properties.	
Various Multi-component Metal Alloys (~6.4 million compositions screened, 6480 promising)	Ensemble Learning Model (within the HEART framework)	Hydrogen storage capacity (H ₂ wt%), Enthalpy of hydride formation (ΔH)	High-throughput virtual screening using ML to identify a large number of potential hydrogen storage materials with desirable properties.	[312]
Various Metal Hydrides (dataset of 1280 metal alloys)	Hybrid Machine Learning Framework (Unsupervised learning using Autoencoder + Supervised learning using Multi-Layer Perceptron)	Hydrogen storage capacity	Applied a hybrid ML approach to predict hydrogen storage capacity, particularly addressing limitations related to data availability and high-dimensional feature spaces.	[319]
Various Metal Hydride Compositions (dataset-driven)	Gradient Boosting Regression Models	Formation enthalpy (of metal hydrides and intermetallic alloys)	Developed ML models to predict formation enthalpy based on composition, highlighting the challenges in predicting for diverse structural types.	[340]
Various Metal Hydrides (dataset from US Department of Energy)	Multiclass Classification Algorithms (Logistic Regression, Decision Forest, Decision Jungle, Neural Network), Regression Algorithms	Optimal materials class for hydrogen storage, Hydrogen weight percent, Heat of formation, Operating temperature and pressure	Used ML for both classification of material classes suitable for hydrogen storage and regression to predict specific hydrogen storage properties based on criteria.	[338]
Various AB ₂ metal hydrides (dataset of 314 pairs)	Random Forest, Multivariate Regression, Support Vector Machine, Regression Tree, Gaussian Process Regression (GPR)	Heat of formation (ΔH), Phase abundance, Hydrogen capacity	Analyzed the effects of alloying elements on the hydrogen storage properties of AB ₂ -type metal hydrides using various ML algorithms.	[321]
Selected HEA hydrides including MgTiVCrNb and MgAlTiVCr	Gradient Boosting Tree Regressors/Classifiers	Hydride stability, Thermodynamic properties (from van't Hoff analysis)	ML predictions guided the experimental synthesis and characterization of specific HEA hydrides to validate their thermodynamic stability.	[322]
TiVZrNbHfHx (benchmark HEA hydride) and novel destabilized HEA hydrides (specific compositions not explicitly listed as a large set)	Compositional Machine Learning Model	Hydride stability (equilibrium pressure, desorption enthalpy)	ML screening was used to identify compositions with targeted thermodynamic stability, leading to the experimental synthesis of novel hydrides with significantly altered properties compared to the benchmark.	[332]

6. Areas for future research direction

Solid-state hydrogen storage using CCAs and HEAs presents a compelling pathway for next-generation energy materials. This is due to their ability to reversibly store substantial hydrogen quantities under ambient conditions. Despite being a relatively nascent field, research interest is growing rapidly due to the potential advantages of CCAs/HEAs such as high storage capacity, structural tunability, and resistance to hydrogen embrittlement (Fig. 25). However, a major challenge remains in balancing hydrogen capacity with favourable absorption/desorption kinetics. This trade-off has not been extensively addressed, yet it is critical for enhancing the performance and practicality of CCA/HEA-based hydrides in real-world hydrogen systems.

To overcome current limitations, future research should prioritize

mechanistic understanding, microstructure–property correlations, and compositional optimization. The complexity of multi-principal element systems often leads to sluggish kinetics and high processing costs, which must be mitigated to enable scalable applications. Computational tools like machine learning and CALPHAD offer powerful means to predict and refine alloy behavior across vast compositional spaces. In parallel, high-throughput experimentation and targeted validation will be essential to accelerate the discovery of HEA hydrides with improved kinetics, lower operating temperatures, and economic viability. Advancing these areas will be pivotal for realizing the role of HEAs in a sustainable hydrogen economy.

The body-centered cubic (BCC) structure has attracted significant interest in high-entropy alloys (HEAs) for hydrogen storage. This is due to its superior hydrogen uptake at room temperature and high storage

Table 8

Different solid state hydrogen storage materials studied using various forms of ML tools with evaluation metrics.

Material Class	Feature Descriptors	Target Properties	Machine Learning Models	Best Model	Evaluation Metrics	Refs
Multi-category HSMs	1) Materials class 2) Temperature 3) Heat of formation 4) Pressure 5) Composition formula	Hydrogen storage capacity	1) LR 2) NN 3) BLR 4) GBDT	GBDT	MAE: 0.003 wt% H ₂ RMSE: 0.012 wt% H ₂ R ² : 0.83	[341]
Multi-category HSMs	1) Hydrogen storage capacity 2) Temperature 3) Heat of formation 4) Pressure	Material class	1) L-R 2) DF 3) DJ 4) NN	NN	Accuracy: 0.8	[338]
Multi-category HSMs	1) Hydrogen storage capacity 2) Temperature 3) Heat of formation 4) Pressure	Similar behaviors of different materials classes	k-means	k-means	Number of clusters: 3 Intra-cluster cohesion: 0.6 Inter-cluster separation: 1.4	[342]
Multi-category HSMs	1) Band gap, 2) Density 3) Atomic volume 4) Magnetization 5) Electronegativity 6) Avg d-character 7) Avg f-character 8) Temperature and 9) Pressure	Formation energy	1) Ridge 2) DT 3) RF 4) GBDT	RF	MSE: 0.102 eV ²	[3]
Multi-category HSMs	Magpie framework	Equilibrium pressure	GBDT	GBDT	MAE _{train} = 0.47 MAE _{test} = 1.52	[343]
Multi-category HSMs	Magpie framework	Hydride formation enthalpy	1) RepTree, 2) RF and 3) NN	RF	MAE = 8.56 kJ/mol, R ² = 0.89 MRRE: 28 %	[344]
Multi-category HSMs	1) Fundamental Properties 2) Interactions-based features 3) Composition-dependent properties and 4) Temperature	1) Hydrogen storage capacity (HYST) 2) Hydride formation enthalpy (THOR)	1) ETR, 2) Ridge, 3) LASSO 4) KRR, 5) GPR 6) RF, 7) ETR 8) GBDT	1) ETR 2) ETR	1. R ² = 0.81 MAE = 0.45 wt% H ₂ 2. R ² = 0.89 MAE = 4.53 kJ/mol H ₂	[312]
Ti-based HSMs (AB ₂ -type)	Constituent elements	1) Hydride formation enthalpy, 2) Phase abundance 3) Hydrogen storage capacity	1) MLR 2) DT 3) RF	RF	1. R ² = 0.647, MAE = 4.36 kJ/mol H ₂ RMSE = 5.75 kJ/mol H ₂ 2. R ² = 0.832, MAE = 22.4 %, RMSE = 25.6 % 3. R ² = 0.688, MAE = 0.101 wt% H ₂ RMSE = 0.159 wt% H ₂	[345]
Ti-based HSMs (AB ₂ -type)	Constituent elements	Hydride formation enthalpy	GPR with different kernels	GPR with Exponential kernel	R ² = 0.969, MRE = 2.291 %, MSE = 3.909 kJ ² /mol ² H ₂ , RMSE = 2.501 kJ/mol H ₂ STD = 1.878 kJ/mol H ₂	[346]
Ti-based HSMs (AB ₂ -type)	Constituent elements	Hydrogen storage capacity	1) GA-LSSVM 2) PSO-LSSVM, 3) HGAPSO-LSSVM	HGAPSO-LSSVM	R ² = 0.980, STD = 0.043 wt% H ₂ MSE = 0.002 wt% H ₂ , RMSE = 0.045 wt% H ₂	[347]
Ti-based HSMs (AB ₂ -type)	Constituent elements	Hydride formation enthalpy	1) MLR, 2) SVM 3) DT, 4) GPR with different kernels	GPR with Exponential kernel	R ² = 0.969, MRE = 2.291 % MSE = 1.18 kJ/mol ² H ₂ , RMSE = 1.09 kJ/mol H ₂ MAE = 0.70 kJ/mol H ₂	[348]
Ti-based HSMs (C14 Laves-type)	1) Magpie framework 2) Constituent elements 3) Atomic radius 4) Hydrogen affinity ability 5) Elemental stoichiometry ratio	1) Cell volume 2) De-/hydrogenation equilibrium pressure (ln P _{H₂} /d _{es}) 3) Hydride decomposition enthalpy 4) Hydrogen storage capacity	1) LR 2) PLR 3) Ridge 4) LASSO 5) SGDR 6) DT 7) RF 8) GBDT 9) SVR 10) MLP	SVR, GBDT	1) R ² = 0.987 Abs: R ² = 0.973 Des: R ² = 0.978 2) R ² = 0.916 4) R ² = 0.822	[349]
Ti-based HSMs (AB ₂ -type, Fitted PCT data)	1) Constituent elements 2) Temperature 3) Pressure	De-/hydrogenation PCT behaviors	1) MLP 2) RF 3) KNN 4) DNN	DNN	R ² = 0.9307	[350]
Solid solution HSMs (V-Ti-Cr-Fe-based)	1) Constituent elements 2) Fundamental properties of elements 3) Temperature	Hydrogen storage capacity	1) LR, 2) LASSO 3) XGBoost 4) BF, 5) SVM 6) Stacking 7) (RF, SVM, XGBoost) 8–11) Adaboost variants	Adaboost Stacking	MSE = 0.187 wt% H ₂ MAE = 0.307 wt% H ₂ R ² = 0.783 PC = 0.885	[351]

(continued on next page)

Table 8 (continued)

Material Class	Feature Descriptors	Target Properties	Machine Learning Models	Best Model	Evaluation Metrics	Refs
Solid solution HSMs (V-Ti-Cr-Fe-based)	1) Constituent elements 2) Fundamental properties of elements and 3) Temperature	Hydride decomposition enthalpy	1) LR, 2) SVM 3) BF, 4) XGBoost 5) Stacking	XGBoost	MAE = 8.58 kJ/mol RMSE = 11.73 kJ/mol $R^2 = 0.783$ and PC = 0.885	[352]
Solid solution HSMs (High entropy alloys)	1) Magpie framework 2) Hydride specific feature	1) Hydrogen storage capacity (H/M) 2) Hydride decomposition enthalpy 3) Hydride decomposition entropy 4) Equilibrium pressure	GBDT	GBDT	1. MAE = 0.12 $R^2 = 0.79$ 2. MAE = 4.2 kJ/mol H ₂ $R^2 = 0.90$ 3. MAE = 11 J/mol-K H ₂ $R^2 = 0.69$ 4. MAE = 1.1 $R^2 = 0.93$	[353]
Solid solution HSMs (High entropy alloys)	1) Magpie framework 2) Binary hydride formation enthalpy	1) Equilibrium pressure 2) Hydride dissociation enthalpy	GBDT	GBDT	1. MAE = 1.4 2. MAE = 5.5 kJ/mol H ₂	[354]
Solid solution HSMs (High entropy alloys)	Structure-based framework (Extracted by GNN)	Formation energy	GNN	GNN	MAE = 3.1 meV/atom	[355]
Solid solution HSMs (High entropy alloys)	Fundamental properties of elements	Hydrogen binding energies for: 1. First 2. Second stages of absorption	1) LR 2) DT 3) GPR	1. GPR 2. GPR	1. MAE = 0.04 eV $R^2 = 0.71$ 2. MAE = 0.04 eV $R^2 = 0.93$	[356]
Mg-based HSMs (Mg-M-H)	Constituent elements	1) Hydrogen storage capacity 2) Dehydrogenation temperature 3) Plateau pressure	ANN	ANN	$R > 0.95$	[357]
Mg-based HSMs (Mg-M-H)	1) Stoichiometric properties 2) Elemental intrinsic characteristics; 3) Atomic number; 4) Elemental thermodynamics 5) Hydrogen storage capacity	Dehydrogenation temperature	1) GBDT 2) RF 3) XGBoost 4) DT	GBDT	$R^2 = 0.95$ RMSE = 29.98 K	[358]
Mg-based HSMs (Mg-Ni-based HSMs)	Discharge capacities in the initial five cycles	Discharge capacities (after the fifth cycle)	ANN	ANN	$R^2 > 0.99$	[359]
Mg-based HSMs	1) Ewald sum matrices 2) Sine matrices 3) System and frames	Formation energy	1) KRR 2) DeePMD	DeePMD	RMSE = 0.43 meV/atom	[360]
Mg-based HSMs (MgH ₂ nanoclusters)	Structure-based framework	1) Energy from DFT 2) Force from DFT	ANN	ANN	1. RMSE = 31.25 meV/atom MAE = 18.23 meV/atom 2. RMSE = 189.9 meV/Å MAE = 95.48 meV/Å Structure validation ratio: 96	[361]
Mg-based HSMs (2D MgH ₂ sheets)	Point-cloud-like image representation of a 2D matrix	Reliability of generated structures	GAN	GAN		[362]
Mg-based HSMs	1) Fundamental properties of elements 2) VEC distributions 3) Thermodynamic parameters 4) Processing conditions	1) Maximum absorption capacity 2) Maximum desorption capacity	1) SVR 2) MLP 3) GBDT 4) RF	1) GBDT 2) MLP	1. MSE = 0.12 wt% H ₂ MAE = 0.24 wt% H ₂ $R^2 = 0.947$ 2. MSE = 0.16 wt% H ₂ MAE = 0.32 wt% H ₂ $R^2 = 0.922$ MAE = 5.5 kJ/mol H ₂	[363]
Mg-based HSMs (Mg-Ni-M ternary intermetallic)	Structure-based framework	Hydride formation enthalpy	MEGNet+ Transfer learning	MEGNet + Transfer learning		[364]
Complex HSMs (LiBH ₄ -based mixture)	1) Catalysts and their ratio 2) Ball milling condition 3) Heating rate	Dehydrogenation kinetic performance	1) LR, 2) Ridge 3) LASSO, 4) MLP, 5) GBDT 6) DT, 7) Ada DT 8) Bagging 9) ETR, 10) RF 11) Hist	EOE (based on DT, GBDT, KNN, MLP)	MSE = 1.144 wt% H ₂ , RMSE = 1.066 wt% H ₂ , EV = 0.889 $R^2 = 0.888$, PC = 0.944 and SC = 0.949	[364]
Complex HSMs (Metal Borohydride)	Structure-based framework	Formation energy	CGCNN	CGCNN	MAE = 0.063 eV/atom	[365]

NB: Machine learning models: LR – Linear Regression; BLR – Bayesian Linear Regression; MLR – Multivariate Linear Regression; L-R – Logistic Regression; KRR – Kernel Ridge Regression; LASSO – Least Absolute Shrinkage and Selection Operator; PLR – Polynomial Linear Regression; SGDR – SGD Regression; DT – Decision Tree; RF – Random Forest; GBDT – Gradient Boosted Decision Tree; Hist – Histogram-based Gradient Boosting Tree; DF – Decision Forest; DJ – Decision Jungle; ETR – ExtraTree Regression; LGBMR – LGBM Regression; SVM – Support Vector Machine; LSSVM – Least Square Support Vector Machine; SVR – Support Vector Regression; NN – Neural Network; ANN – Artificial Neural Network; MLP – Multilayer Perceptron; BPNN – Back Propagation Neural Network; GNN – Graph Neural Network; CGCNN – Crystal Graph Convolutional Neural Network; GAN – Generative Adversarial Network; MEGNet – Materials Graph Network; DeePMD – Deep Potential Molecular Dynamics; SSCHA – Stochastic Self-Consistent Harmonic Approximation; GPR – Gaussian Process Regression; GA – Genetic Algorithm; PSO – Particle Swarm Optimization; HGAPSO – Hybrid GA-PSO.

Table 9

Evaluation metrics used for the estimating the error functions in hydrogen storage materials studied using machine learning models [3].

Metric and relevant equation	Optimal value	Use case
$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$	1.0	Assessing the accuracy of hydrogen leak detection systems
$Precision = \frac{TP}{TP + FP}$	1.0	Evaluating the precision of sensors detecting hydrogen purity
$Recall \text{ (Sensitivity)} = \frac{TP}{TP + FN}$	1.0	Measuring the ability to detect hydrogen leaks accurately
$F1 - \text{Score} = \frac{2 \cdot \frac{Precision \cdot Recall}{Precision + Recall}}$	1.0	Balancing precision and recall in hydrogen purity analysis
$\text{Mean Absolute Error (MAE)} = \frac{1}{n} \sum_{i=1}^n y_i - \hat{y}_i $	0	Forecasting hydrogen production rates
$\text{Mean Squared Error (MSE)} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$	0	Predicting the energy consumption in hydrogen generation
$\text{Root Mean Squared Error (RMSE)} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}$	0	Evaluating the precision of hydrogen storage level forecasts
$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$	1.0	Assessing the fit of models predicting hydrogen production efficiency
$\text{Mean Reciprocal Bank (MRR)} = \frac{1}{ Q } \sum_{i=1}^{ Q } \frac{1}{rank_i}$	1.0	Ranking the effectiveness of hydrogen storage methods
$\text{Mean Absolute Percentage Error (MAPE)} = \frac{100\%}{n} \sum_{i=1}^n \left \frac{y_i - \hat{y}_i}{y_i} \right $	0	Predicting hydrogen demand over time

Evaluation metrics: MSE – Mean Squared Error; MRE – Mean Relative Error; MAE – Mean Absolute Error; RMSE – Root Mean Squared Error; R – Correlation Coefficient; R^2 – Coefficient of Determination; STD – Standard Deviation; YN – Residual Standard Error; MAPE – Mean Absolute Percentage Error; PC – Pearson Correlation; SC – Spearman Correlation; EV – Explained Variance.

capacity [3–7,26,43,52,164,165,371]. Achieving a stable BCC phase typically requires a valence electron concentration (VEC) below 6.87, easily predicted using CALPHAD methods [96,372–381]. Beyond VEC, enthalpy, entropy, and atomic size mismatch should also be considered for predominantly BCC structures [24,72,96,114,115,118,148,269,382–387]. Alloys with BCC structures have demonstrated hydrogen-to-metal (H/M) ratios up to 2, and vanadium-rich compositions exceeding 30 % V have shown capacities up to 3.5 wt% under mild conditions [388–390]. However, these systems often suffer from slow hydrogen absorption and desorption kinetics, limiting their practical applications [391]. Hence physics-based ML and high throughput computational screening are required to avoid compositionally restrictive spaces and microstructural tuning in CCAs/HEAs [392–394]. This has been proven in Ti-V-Nb-Cr system where C15 Laves phase were varied within the BCC matrix. In Ti22V22Nb22Cr33 alloy with 3 % Laves phase, 3 wt% H/M capacity was achieved, whereas ~8 % Laves phase in Ti11V30Nb28Cr31 resulted in enhanced kinetics with H/M capacity of 2.5 wt% [395]. Although, there was trade-off between kinetics and storage capacity influenced by microstructural tuning, rational alloy design based on multiple optimization framework could provide an ideal composition-processing-microstructure combination to overcome intrinsic or extrinsic trade-offs.

Achieving intrinsic activation mechanisms in CCAs/HEA-based for hydrogen uptake is another area for investigation. This process could eliminate the need for external activation which has mechanistic drawbacks and cost implications. Current external or traditional activation strategies such as high-pressure torsion or thermal treatments improve hydrogen uptake but introduce addition processing complexity. Future research should explore the development of self-activating

Table 10

Typical databases for ML-based prediction for hydrogen storage applications.

Materials class	Data entries	Materials properties	Data Source	Refs
Multi-category HSMs (HydrPARK)	2722	Hydrogen storage capacity and Heat of formation	HydPARK	[366]
Multi-category HSMs (ML-HydrPARK)	398	Hydrogen storage capacity, Heat of formation, Entropy of formation and Equilibrium pressure	ML-Hyd rPARK_000	[326,332, 336–338, 343]
	400		ML-Hyd rPARK_001	
	428		ML - Hyd rPARK_002	
	429		ML - Hyd rPARK_003	
	430		ML - Hyd rPARK_004	
	772		ML - Hyd rPARK_005	
Complex and high-density HSMs	2150	Heat of formation, Phase abundance and Hydrogen storage capacity	High density HSMs	[3]
AB ₂ -type HSMs	314	Hydride formation enthalpy, Hydride formation entropy, Phase abundance and Hydrogen storage capacity	AB ₂ - Type HSMs	[321]
AB ₅ -type HSMs	420	Hydrogen formation and Hydride formation enthalpy	AB ₅ - Type HSMs	[322]
Mg-based HSMs (DFT data)	15295	Formation energy	Mg-based HSMs (DFT)	[367]
Mg-based HSMs	636	Heat of Hydride formation and Equilibrium potential	Mg-based HSMs	[368]

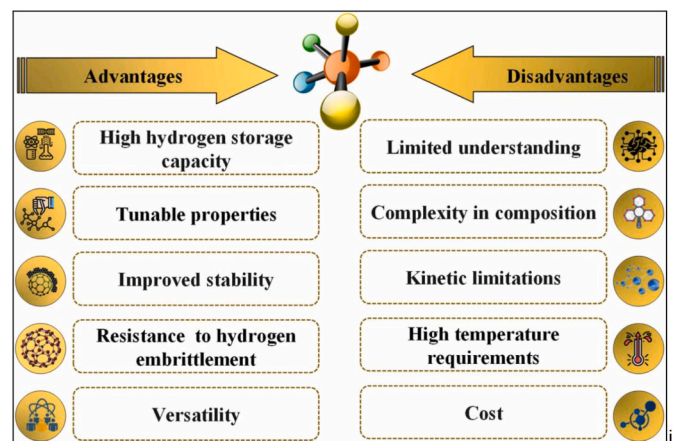


Fig. 25. Summary of the advantages and disadvantages of HEAs for hydrogen storage underscoring the need for further research [33].

HEAs/CCAs through tailored composition and microstructure. This could involve incorporating elements with strong hydrogen affinity (e. g., Ti, V, Ce) which inherently promote hydrogen absorption and minimize oxidation. Additionally, defect engineering approaches, such as severe plastic deformation or high-energy ball milling, can introduce high densities of grain boundaries and dislocations to serve as fast diffusion pathways for hydrogen. Designing such self-activating systems could eliminate pre-treatment steps and significantly advance the practical viability of HEA-based hydrogen storage materials.

The multifaceted challenges associated with hydrogen energy and storage applications are summarized in Fig. 26. These are categorized

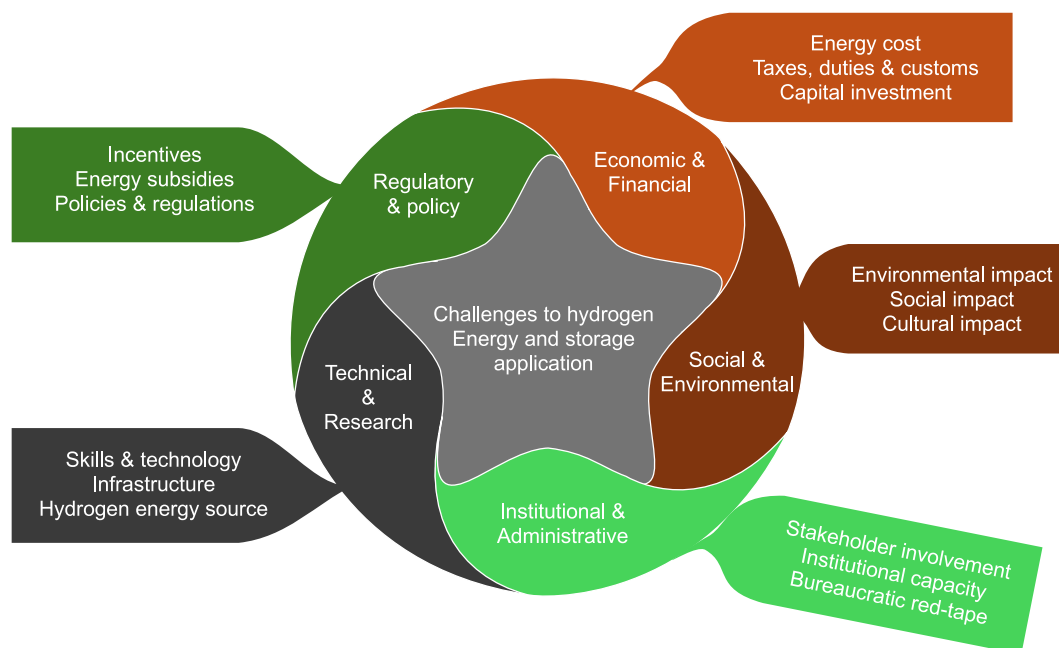


Fig. 26. Barriers and challenges to renewable energy deployment [396].

into five primary domains: economic and financial; social and environmental, institutional and administrative; technical and research; and regulatory and policy challenges. At the core of the research gaps identified, lies the acknowledgment that successful hydrogen energy storage and technology adoption requires addressing all the interconnected areas simultaneously and synergistically. Each domain highlights specific barriers ranging from financial hurdles like energy costs and capital investment to social considerations such as environmental and cultural impacts which must be navigated to enable a viable hydrogen economy.

There are external forces shaping the hydrogen energy and storage technology adoption. The notable ones include economic and financial sectors as well as the social and environmental sectors which are critical in driving sustainability indicators. High energy costs, complex tax structures, and the need for significant upfront investments can deter stakeholders from committing to hydrogen infrastructure. Simultaneously, societal acceptance is influenced by the perceived environmental benefits or harms, social equity concerns, and cultural attitudes toward new energy technologies. These issues are deeply intertwined: without public support and feasible financial models, even the most technically sound hydrogen solutions risk stagnation or rejection.

The technical know-how is anchored by research and institutional and administrative challenges coupled with regulatory and policy domains does reflect the internal mechanisms to operationalise hydrogen energy strategies. Technical advancements in hydrogen production, storage, and infrastructure must be supported by strong institutional frameworks and streamlined administrative processes that minimize bureaucratic inefficiencies. Effective regulatory policies through incentives, subsidies, and clear regulations can further accelerate hydrogen deployment. Thus, Fig. 26 maps the obstacles and also implies that an integrated, multi-sectoral effort is critical for overcoming the complex ecosystem of challenges in hydrogen energy development.

Furthermore, critical opportunities for future research and innovation are highlighted. Each domain be it economic, social, institutional, technical, and regulatory presents specific gaps that, if strategically addressed, could accelerate the transition toward a sustainable hydrogen economy. By systematically exploring solutions to reduce energy costs, enhance public acceptance, streamline institutional processes, advance technical capabilities, and refine regulatory

frameworks, researchers and policymakers can collaboratively shape the future of hydrogen technologies. Thus, the challenges outlined could serve as a roadmap for targeted research, offering a rich landscape for interdisciplinary inquiry and impactful advancement.

7. Conclusions

This study conducted a bibliometric analysis of the literature on HEAs as hydrogen storage materials from 2010 to May 30, 2024. A total of 214 research articles were extracted from the Scopus database and analyzed using VOSviewer software. The leading journals in this field are the International Journal of Hydrogen Energy, Journal of Alloys and Compounds, and Inorganic Chemistry, which rank as the top three contributors to research on hydrogen storage with HEAs.

China and its institutions dominate in terms of publications and contributions to this area, reflecting a strong commitment to advancing HEA research. Furthermore, network mapping of co-occurring author keywords has revealed current trends and suggested future research directions, including the application of machine learning, optimizing the balance between hydrogen storage capacity and kinetics, and enhancing our understanding of hydrogen storage mechanisms, all of which warrant further exploration.

The paper illustrates the great strides which have been taken in HEA metal hydrides from their inception in 2010 wherein HEA metal hydrides move from storage capacities of 1.3 wt% in Kao et al.'s initial work to high of 3.7 wt% in Chen et al.'s contribution to HEA metal hydrides. 2016 produced the highest cited paper in the field to date as Sahlberg et al. produced TiZrNbHfTa metal hydride which exhibited an unprecedented 2.5 H/M at room temperature which is considered as remarkable hydrogen storage performance which generated great interest with the field which is shown by the gradual increase yearly.

The most popular synthesis method used in manufacturing HEA metal hydrides is Arc melting, this is due to its ability to melt at high temperatures, ability to produce HEA with homogeneity and prevention of contamination by means of vacuum melting environment. However, the design and manufacturing of HEA metal hydrides has been simplified using machine learning and computational modelling tools that assist in predicting, designing and producing suitable HEA metal hydrides.

Even though the field is relatively young and is still to generated large scale interest, the potential for HEA metal hydrides is high as their ability to storage large amounts of hydrogen at room temperature while having low desorption temperatures can assist in manufacturing metal hydrides that meet the US DOE targets for commercially viable metal hydrides that can push the hydrogen economy forward.

The insights gained from this bibliometric and systematic review provide a solid foundation for understanding HEA metal hydrides, current trends, and future research opportunities. Expanding research initiatives and promoting international collaboration will be essential for improving the feasibility of HEAs as commercially viable metal hydrides for hydrogen storage applications.

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.

Data availability

Data will be made available on request.

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