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Invited review

Review of hydrogen storage modeling and simulations

Junming Lao[1], Zhenhuan Xie[1], Yiyang Zhou[1], Shuyi Du[1], Weiyao Zhu[1], Hongqing Song[1]*

[1]*School of Civil and Resource Engineering, University of Science and Technology Beijing, Beijing 100083, P. R. China*

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Abstract:
Hydrogen storage is pivotal in the hydrogen industry chain by buffering the extensive hydrogen production from upstream and stabilizing the downstream hydrogen supply, underpinning the global efforts against global warming and extreme climate. Modeling and simulation are imperative approaches to evaluate and predict the reliability of hydrogen storage schemes and prevent repeated costly experiments. Therefore, we perform a critical review on the developments and explorations of hydrogen storage modeling and simulation in the last decade. The review is divided into two themes, where first we review the hydrogen storage schemes, specifically underground hydrogen storage, solid material hydrogen storage, high pressure compression storage and fuel cell on-board storage. Then we review modeling and simulation methods, including hybrid energy system assessments, thermodynamics, molecular dynamics and machine learning. Last but not least, we summarize the research focuses of modeling and simulation in hydrogen storage, clarify the current challenges and propose the future research topics. We undertake this work to advance the explorations of hydrogen storage modeling and simulation and drive the creativity on addressing the current hydrogen storage shortages.

1. Introduction

The significance of hydrogen as a sustainable and clean energy carrier is widely recognized, underpinning the global efforts towards decarbonization and energy transition (Abdalla et al., 2018; Abe et al., 2019; Song et al., 2021). Hydrogen storage emerges as a crucial technology in this landscape, enabling the effective utilization of hydrogen in various applications, including power generation, transportation, and as a buffer for renewable energy sources (Lao et al., 2021a, 2023b). The ability to store hydrogen efficiently addresses the intermittent nature of renewable energies and facilitates the integration of hydrogen into the existing energy infrastructure, underscoring the significance of advancing hydrogen storage solutions.

Modeling and simulation have become indispensable tools in hydrogen storage research, offering insights into the complex physical and chemical processes underlying various storage methods (Muhammed et al., 2022; Usman, 2022; Krevor et al., 2023). These computational approaches enable the exploration of material properties, system designs, and operational strategies without the extensive costs and time associated with empirical testing. Through modeling and simulation, researchers can predict the behavior of hydrogen storage systems under different conditions, optimize material compositions for higher storage capacities and kinetics, and evaluate the integration of storage solutions with renewable energy systems.

The functions of modeling and simulations are diverse, spanning underground hydrogen storage, solid material storage (such as metal hydrides, metal-organic frameworks (MOFs), and graphene/carbon nanomaterials), high-pressure compression storage, and fuel cell on-board storage. Each of these storage schemes presents unique challenges and opportunities for optimization. For instance, underground hydrogen storage offers prospects for large-scale, long-term energy storage, necessitating models to assess geological suitability and environmental impacts. Solid material storage relies on the physicochemical interactions between hydrogen and the storage medium, where simulations help in designing materi-

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*Corresponding author.
E-mail address: junminglao@ustb.edu.cn (J. Lao); U202240110@xs.ustb.edu.cn (Z. Xie); D202310003@xs.ustb.edu.cn (Y. Zhou); 15702449699@163.com (S. Du); weiyaook@sina.com (W. Zhu); songhongqing@ustb.edu.cn (H. Song).
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als with enhanced hydrogen adsorption/desorption properties. High-pressure and cryogenic storage systems benefit from modeling efforts to improve safety, efficiency, and materials compatibility. Fuel cell on-board storage models focus on integrating hydrogen storage with fuel cell systems to maximize energy density and minimize refueling time for transportation applications.

Current modeling and simulation methods range from molecular dynamics and thermodynamics simulations for material analysis to pore and field scale simulations for evaluating the performance and safety of storage solutions. Machine learning and big data analytics have also emerged as powerful tools, offering new avenues for predicting material properties and optimizing storage systems. These methods collectively contribute to a deeper understanding of hydrogen storage mechanisms, material behavior under storage conditions, and the integration of storage systems with broader energy infrastructures.

In the realm of hydrogen storage, modeling and simulation serve as critical enablers, providing the necessary insights and tools to overcome technical challenges and unlock new potentials. The ongoing advancements in computational techniques and the growing repository of simulation data are propelling the field towards innovative solutions that promise to enhance the viability and efficiency of hydrogen storage technologies. As we continue to explore and refine these computational approaches, the prospects for achieving scalable, sustainable, and economically feasible hydrogen storage solutions become increasingly tangible, marking a significant stride towards a hydrogen-powered future.

Here, we review the developments and explorations of modeling and simulation on hydrogen storage and provide an in-depth insight of current challenges and future research topics. The themes we review are exhibited in Fig. 1. Sections 2 to 5 review the hydrogen storage schemes, specifically underground hydrogen storage, solid material hydrogen storage, high pressure compression storage and fuel cell on-board storage. Section 6 to 9 review modeling and simulation methods, including hybrid energy system assessments, thermodynamics, molecular dynamics and machine learning. A fraction of references may fall in several sections of this review. In this case, we configure those papers in the most related topic. In section 10, we discuss the significance of modeling and simulation in hydrogen storage research, clarify the current challenges and propose the future research topics. Eventually we summarize this review in the conclusion section.

2. Underground hydrogen storage

2.1 Long-term and large-scale storage potential

The transition towards renewable energy sources necessitates innovative solutions for energy storage, with hydrogen emerging as a pivotal component due to its versatility and sustainability. The integration of renewable energies into our current systems presents a significant challenge, notably in balancing supply and demand over varying time scales. Seasonal storage solutions, as explored by Reuß et al. (2017), offer a path forward, emphasizing the need for a flexible hydrogen supply chain that can adapt to the fluctuating nature of renewable energy production.

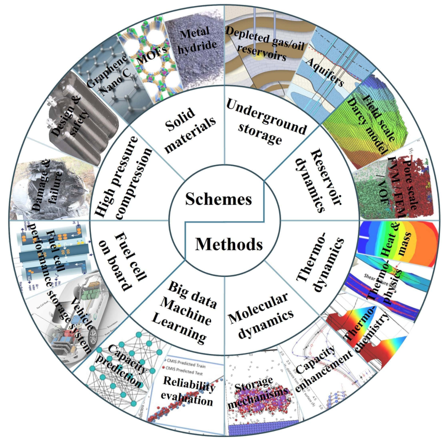


Fig. 1. Schematic illustration of the modelling and simulation research on hydrogen storage.

The potential for underground hydrogen storage (UHS) as a large-scale solution has garnered increasing attention. Ceran et al. (2021) and Zeng et al. (2022) have analyzed and proved the viability of UHS as a long-term and large-scale hydrogen storage solution. These studies underscore the importance of identifying favorable geological conditions and understanding the operational challenges, including aging effects on the infrastructure's performance. Liu et al. (2024) numerically investigated the feasibility of hydrogen storage in depleted shale gas reservoirs, inspired by the mechanisms uncovered from Song et al. (2023c), can be seen in Fig. 2(a).

Moreover, the long-term and large-scale storage potential of hydrogen is a key component in the transition to renewable energy sources. This necessitates a comprehensive analysis, as suggested by Pfeiffer and Bauer (2019) and Abdellatif et al. (2023), to ensure the feasibility and reliability of UHS in meeting the demands of large-scale energy storage. Lao et al. (2021a, 2023b) and Song et al. (2021) have explored a capacity assessment model of hydrogen storage in depleted oil reservoir for uptaking offshore wind power and proved their scheme is profound by matching the field data, as illustrated in Fig. 2(b)

Herein, through a combination of underground storage and a comprehensive understanding of the challenges involved, hydrogen storage can provide the flexibility and stability needed to integrate renewable energies into our energy systems effectively.

2.2 Field and pore scale simulations

Field and pore-scale simulations play a crucial role in advancing our understanding of UHS, focusing on the potential for utilizing various geological formations for safe and effective storage solutions. Hemme and van Berk (2018) have made significant contributions through hydrogeochemical modeling, identifying geological formations that promise safety and environmental compatibility for UHS. Building on this foundation, Chabab et al. (2020) provided valuable measurements and predictive models of hydrogen solubility in brines at high pressures, which are essential for evaluating both the capacity and integrity of storage sites.

For field scale investigations, Hassannayebi et al. (2019) furthered this exploration by applying geomechanical simulations to assess the feasibility of UHS in depleted gas fields, showcasing the potential for repurposing existing geological infrastructures for hydrogen storage. Their work supports the strategic development of hydrogen infrastructure by evaluating geological formations for their storage capabilities. Pfeiffer et al. (2016) examined hydrogen storage in synthetic large-scale underground facilities, highlighting the immense potential of geological formations for massive energy storage.

In pore scale and micro scale, Hagemann et al. (2015) delved into the challenges of hydrogen transport in porous media, focusing on the unstable transport phenomena that are critical to ensuring the safety and efficiency of UHS solutions. Bagheri et al. (2023) and Wang et al. (2023) performed direct pore-scale simulation of the effect of capillary number and gas compressibility on cyclic underground hydrogen storage and production in heterogeneous aquifers, providing a comprehensive pore-scale cognition of hydrogen transport properties in deep saline aquifers.

The molecular dynamics simulations conducted by Cai et al. (2022) and Ghasemi et al. (2022), which provided deeper insights into hydrogen diffusion in underground formations, and the development of novel simulators for UHS modeling, have explicated complemented insights to the field scale and pore scale research. These studies collectively offer a comprehensive understanding of the field and pore-scale dynamics governing hydrogen storage in geological formations, marking a significant step toward harnessing this potential for grid-scale energy storage.

The body of work from these researchers emphasizes not only the technical feasibility but also the environmental considerations and safety protocols necessary for implementing UHS solutions. By addressing the barrier of hydrogen permeation in pipelines, as discussed by Ozturk et al. (2016), and exploring subsurface geological formations for their storage potential, this research contributes to the strategic and safe development of hydrogen storage infrastructure.

3. Solid material hydrogen storage

3.1 Metal hydride

Metal hydrides represent a pivotal area in hydrogen storage technologies, offering a blend of high storage density and the potential for reversible hydrogen adsorption and desorption processes. The development and optimization of metal hydride storage systems are critical for enabling effective hydrogen storage solutions, necessitating advanced modeling and simulation techniques to understand and enhance these complex interactions.

The $LaNI_5$ metal hydride system becomes popular and attain extensive attention. Chandra et al. (2020) delve into the modeling and simulation of hydrogen absorption dynamics within a $LaNi_5$ metal hydride system, shedding light on the intricate processes governing hydrogen storage and release. This foundational work is complemented by Oliva et al. (2018), who bridge experimental findings with theoretical models to explore hydrogen storage in $LaNi_5$-xSnx alloys, pushing the boundaries of metal hydride storage capacities.

The research community has also focused on enhancing the efficiency and safety of metal-hydrogen storage tanks. Mohammadshahi et al. (2016) introduce an improved model focusing on the nuanced metal-hydrogen interactions, aiming to elevate storage efficiency and predictability. In parallel, efforts by Shaji and Mohan (2018) to improve thermal conductivity in metal hydride alloys using copper and nickel additives signal advancements in heat transfer and storage efficiency, crucial for the practical application of these systems. Wood et al. (2020) propose a predictive model incorporating complex physics, real structures and optimized assumptions for nanoscale metal hydride evaluations, as displayed in Fig. 3(b).

Furthermore, the exploration of alkali metal hydrides by Hayes and Goudy (2015) and the investigation of $LaNi_5$-based storage systems by Afzal et al. (2022) exemplify the broadening scope of research aimed at optimizing design and thermal management for more effective hydrogen storage. These studies collectively underscore the significant role of metal hydrides in the hydrogen storage ecosystem, highlighting the ongoing innovations and challenges in harnessing these materials for energy storage applications.

Overall, the current research underscores the rigorous investigation and modeling efforts dedicated to enhancing metal hydride hydrogen storage systems. Through improved understanding of material interactions, thermal management, and storage mechanisms, researchers are paving the way for more efficient, safe, and scalable hydrogen storage solutions.

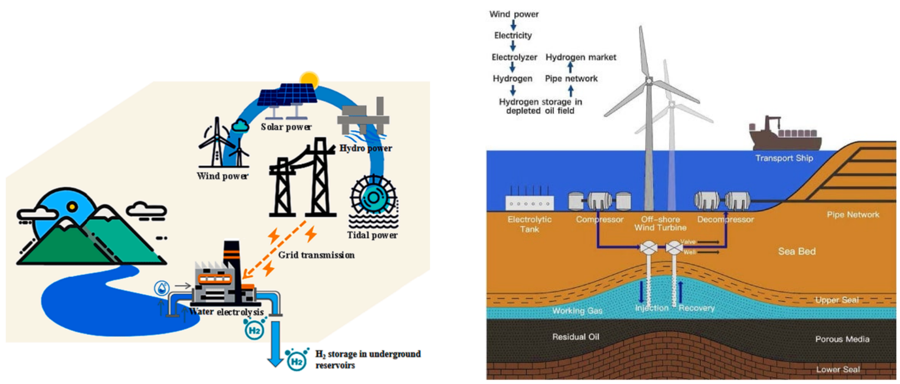
3.2 Porous materials for hydrogen storage

3.2.1 Metal organic framework (MOF)

MOFs have emerged as a forefront in hydrogen storage technology due to their unique properties, including high surface areas, tunable pore sizes, and the ability to modify the framework for specific applications. This section delves into the advancements in modeling and simulations that have propelled MOFs to the forefront of hydrogen storage solutions.

Kocman et al. (2015) further this exploration by analyzing the effectiveness of density functionals in modeling hydrogen adsorption energies within MOFs, a critical step for accurate performance prediction. Basdogan and Keskin (2015) underscore the simulation and modeling efforts that reveal the potential of MOFs due to their high surface areas and customizable porosity, displayed in Fig. 3(a). Cao et al. (2021) highlight the potential and limitations of MOFs in hydrogen storage, respectively, with a focus on their high surface areas, tunable properties, and the challenge of idealized models in capturing the true behaviors of these materials at the nanoscale.

Expanding on this foundation, Andersson and Larsson (2016) and Lu et al. (2022) showcase studies on MOFs' adsorption properties, emphasizing the role of computational methods in material design and the consideration of thermal effects on storage performance by Lindoy et al. (2015). Liu et al. (2022)'s investigation into MOF/graphene oxide composites for hydrogen storage introduces the concept of material



(a) (b)

Fig. 2. (a) Schematic of the Underground Hydrogen Storage in Reservoirs for large-scale and long-term renewable energy storage (Song et al., 2023c). (b) Schematic diagram and workflow of the hybrid energy system (Song et al., 2021).

synergy, enhancing storage characteristics by combining the strengths of different materials.

New material explorations inspired by properties of MOFs illustrate a promising realm in solid material hydrogen storage. Mondal et al. (2022)'s study on the hydrogen storage capacity of Zirconium-based frameworks and Wu et al. (2014)'s introduction of new porous aromatic frameworks further illustrate the diversity and potential of MOFs and related materials in addressing the challenges of efficient hydrogen storage.

The collective efforts of researchers in the field of MOFs for hydrogen storage underscore the significant advancements made in understanding and optimizing these materials for energy storage applications. Through a combination of molecular modeling, machine learning, and practical innovations, MOFs stand as a promising solution to the challenges of hydrogen storage, with ongoing research poised to further enhance their efficiency and applicability.

3.2.2 Graphene and carbon nanomaterial storage

Graphene and carbon nanomaterials have emerged as highly promising materials for hydrogen storage, thanks to their exceptional surface area, structural stability, and unique electronic properties. This section highlights key advancements in the modeling and simulation of hydrogen storage capabilities within these materials, showcasing their potential and addressing the challenges faced.

Mahamiya et al. (2022) explore Scandium-decorated C_{24} fullerenes, utilizing density functional theory to unveil their high capacity and stability for hydrogen storage. This study exemplifies the role of transition metals in enhancing adsorption properties. Similarly, Liu et al. (2018) demonstrate the potential of graphdiyne through density functional theory simulations, focusing on its structural stability and favorable hydrogen adsorption characteristics, pointing to the structural advantages of carbon-based materials.

Further exploration by Gao et al. (2021) into Li-decorated B2O monolayers reveals the significance of lithiation in boosting hydrogen storage efficiency, while Dhar et al. (2018) illustrate the innovative use of cellulose nanocrystal templated graphene nanoscrolls, emphasizing their unique structural properties conducive to hydrogen adsorption.

The research extends into the strategic modification of graphene for enhanced storage capabilities, as shown by Kag et al. (2021) and Chakraborty et al. (2022a), who investigate the effects of strain, defect engineering, and metal decoration on hydrogen storage potential, displayed in Fig. 3(c). These modifications aim to create high-capacity storage solutions by leveraging the intrinsic properties of graphene and related materials.

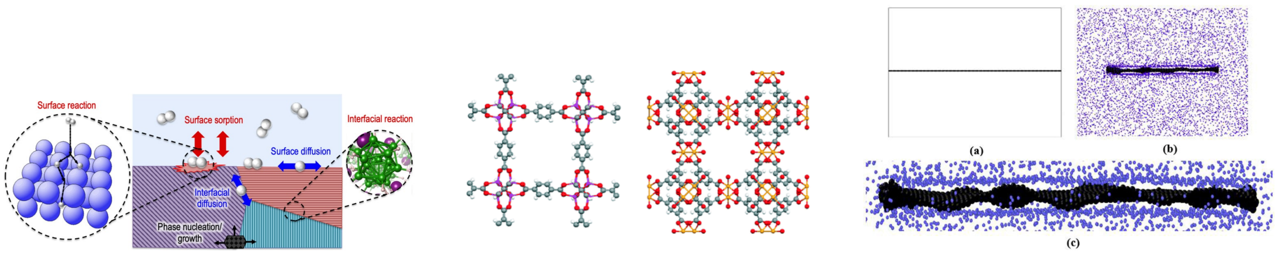
Krylova et al. (2020)'s investigation into crumpled graphene highlights the impact of morphological alterations on storage capacity, demonstrating that structural modifications can significantly enhance hydrogen storage. This is supported by the work of Simagina et al. (2017), which looks into ammonia borane as a solid hydrogen carrier, emphasizing the material's dehydrogenation properties and its potential synergy with carbon nanomaterials.

Further studies, such as those by Tokarev et al. (2015) and Mane et al. (2022b), delve into the enhancement of hydrogen storage in boron-substituted graphene and graphitic carbon nitride, respectively, decorated with alkali metals, showcasing the beneficial interaction between hydrogen and modified carbon surfaces.

The collective research on graphene and carbon nanomaterials for hydrogen storage underscores the significant potential of these materials, driven by their exceptional properties and the innovative strategies employed to optimize their storage capabilities. Through detailed modeling and simulation efforts, researchers are progressively overcoming the challenges of hydrogen storage, paving the way for the development of efficient and high-capacity storage systems based on carbon nanomaterials.

4. High pressure storage and material damage models

Ensuring the structural integrity and performance of hydrogen storage systems, especially under high-pressure conditions, is essential for their safe and efficient operation. Advanced numerical simulations, innovative design method-



(a) (b) (c)

Fig. 3. (a) Schematic illustration of some of the key surface and interface processes taking place during cycling of a typical nanoscale metal hydride material (Wood et al., 2020). (b) Unit cell crystal structure of IRMOF-1 viewed along the [100] direction (left) Zn: violet, O: red, C: gray and H: white. Unit cell crystal structure of CuBTC viewed along the [100] direction (right) Cu: orange, O: red, C: gray and H: white (Basdogan and Keskin, 2015). (c) Adsorbed hydrogen molecules over graphene (Kag et al., 2021).

ologies, and the development of novel storage solutions have significantly contributed to addressing the challenges associated with high-pressure hydrogen storage. Research by Simonovski et al. (2015) and Ye et al. (2020) has been instrumental in optimizing the design and safety of metal hydride hydrogen storage tanks through thermal management and structural integrity assessments, illustrated in Fig. 4(a). Zhang et al. (2020) and Liu et al. (2021) further these advancements with innovative design methodologies for lightweight and safe hydrogen storage vessels, highlighting the importance of balancing efficiency with safety, as shown in Fig. 4(b).

Addressing material damage and failure is another critical aspect of ensuring the reliability and safety of hydrogen storage systems. The development and application of a damage model for 700 bar Type IV high-pressure hydrogen storage vessels by Ramirez et al. (2015a, 2015b, 2015c) mark a significant leap in understanding material behavior under extreme storage conditions, can be seen in Fig. 4(c). This work, along with predictive modeling tools developed by Nguyen et al. (2021), contributes significantly to analyzing damage in composite high-pressure hydrogen storage tanks, enhancing our capability to foresee and mitigate potential failures in storage systems.

The design and safety evaluations of hydrogen storage systems underscore the need for a comprehensive approach to develop predictive models, assess materials and designs, and evaluate the safety of these systems. Efforts by Yersak et al. (2017) to address depressurization-induced icing at hydrogen fueling stations, and by Halm et al. (2017) to evaluate the performance and safety of composite pressure vessels, emphasize the pivotal role of material selection and structural design. Furthermore, the development of physical models by Molkov et al. (2019) to simulate the thermal behavior and safety aspects of onboard hydrogen storage tanks, and lumped parameter simulations by Xiao et al. (2017) for exploring hydrogen storage in metal hydrides, provide valuable frameworks for understanding the intricate balance between storage efficiency and safety.

Collectively, these studies highlight the critical importance of structural integrity, performance, and safety in the development of efficient hydrogen storage solutions. Through rigorous research and innovative design, significant strides have been made in overcoming the challenges associated with hydrogen storage, contributing to the broader adoption of hydrogen as a key energy carrier in a sustainable energy future. The advancements in material damage models and safety evaluations, coupled with the interdisciplinary approach required for hydrogen storage technologies, pave the way for developing reliable, efficient, and safe hydrogen storage systems, underscoring their integral role in sustainable energy systems.

5. Fuel cell and on-board storage

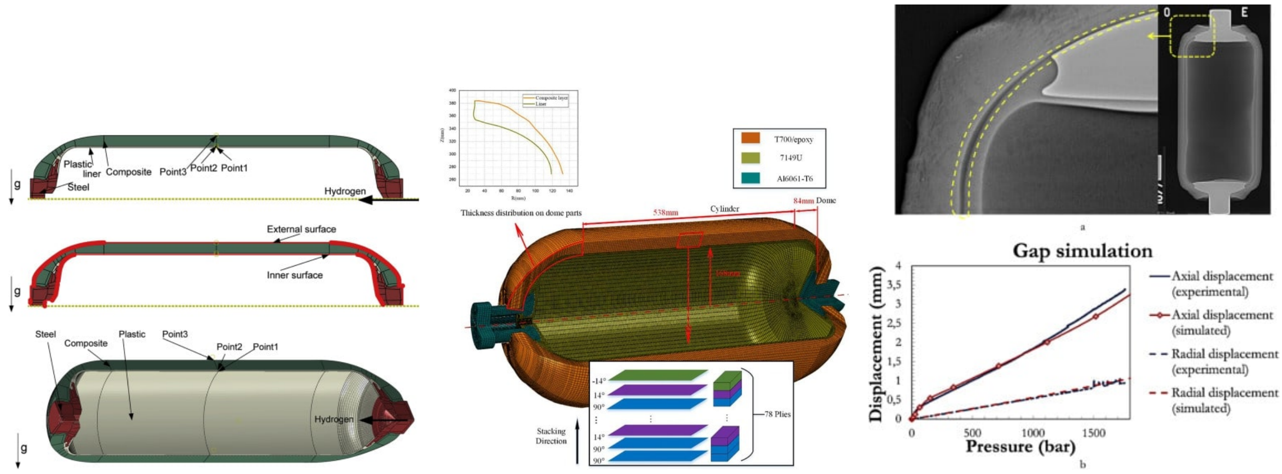
Fuel cells, particularly proton exchange membrane fuel cells, represent a critical technology in harnessing hydrogen for clean energy applications, with on-board hydrogen storage being a key component for transportation. This section reviews significant advancements in fuel cell technology and on-board storage solutions, addressing the challenges and opportunities present in this field.

Ratnakar et al. (2020) delve into hydrogen as an alternative fuel source, discussing the broader context of its storage and transportation challenges. Their work sets the stage for understanding the need for efficient on-board storage solutions to make hydrogen fuel cells viable for vehicles.

Aruna and Christa (2020) present a sophisticated approach to enhancing the operational stability and efficiency of proton exchange membrane fuel cells through mathematical modelling and system identification. Their contributions are vital for optimizing fuel cell performance, ensuring reliable and consistent power output for hydrogen-powered vehicles.

Guarnieri et al. (2015) explore the performance of hydrogen-oxygen unitized regenerative fuel cells, showcasing the potential for these systems to independently size power and energy for effective storage and release, can be seen in Figs. 5(a) and 5(b). This highlights the versatility of fuel cells in energy storage and generation, marking a significant step toward integrated energy systems that can meet varied demands.

The integration of fuel cell technology with on-board



(a) (b) (c)

Fig. 4. (a) 2D axisymmetric and 3D finite element models (Simonovski et al., 2015). (b) Finite element model of a type IV hydrogen storage vessel (Zhang et al., 2020). (c) X-ray micrography: gap location displacement simulation with introduction of a gap (Ramirez et al., 2015a, 2015b, 2015c).

hydrogen storage presents a promising avenue for the development of zero-emission vehicles. Through the contributions of Guarnieri et al. (2015), Aruna and Christa (2020) and Ratnakar et al. (2020), we see a comprehensive approach to overcoming the technical challenges associated with hydrogen storage and fuel cell efficiency. These advancements not only pave the way for cleaner transportation options but also underscore the importance of continued innovation in fuel cell technology and hydrogen storage solutions. As this field evolves, it is imperative to focus on enhancing the efficiency, safety, and economic viability of these systems to ensure their success in the market.

6. Renewable energy integration and hybrid systems

6.1 System design and optimization

The design and optimization of hydrogen storage systems, particularly in the context of renewable energy integration, present complex challenges that require innovative solutions. This section encapsulates the efforts of researchers to address these challenges, highlighting the advancements made towards efficient, reliable, and sustainable hydrogen energy systems.

Trifkovic et al. (2014) tackle the integration and control challenges of renewable hybrid energy systems incorporating hydrogen storage. Their strategies for optimizing system performance amidst the intermittency of renewable sources underscore the need for adaptable and robust system designs. Garcia-Torres et al. (2016) delve into the optimal operation of hydrogen-based microgrids, integrating renewable energy sources to improve efficiency and reliability. Their emphasis on load sharing in real operational scenarios provides valuable insights into the practicalities of hydrogen energy system management.

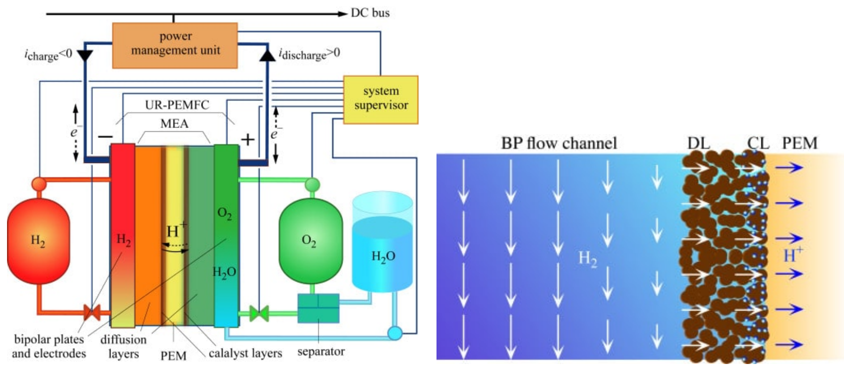
Zhang and Wan (2014) explore a wind-hydrogen energy storage system model, demonstrating its role in grid stabilization and the enhanced penetration of wind energy. This showcases the synergy between renewable energy sources and hydrogen storage solutions, highlighting the potential for such systems to contribute significantly to energy sustainability. Kavadias et al. (2018) model and optimize a hydrogen-based renewable energy system for remote areas, aiming at sustainable and autonomous energy supply, illustrated in Fig. 6(a). Their work aligns with European Union climate and energy targets, illustrating the global relevance of optimized hydrogen storage solutions in achieving energy independence and sustainability.

Further studies, including those by Komiyama et al. (2015), Seo et al. (2020) and Zeng et al. (2023), extend the discourse on system design and optimization, displayed in Fig. 6(b). These studies focus on enhancing the efficiency and sustainability of the hydrogen supply chain, optimizing grid integration of variable renewable sources with hydrogen storage, and the holistic optimization of renewable hydrogen production, storage, and utilization systems, respectively.

Collectively, the research efforts outlined in this section emphasize the critical importance of system design and optimization in the development of hydrogen energy systems. By addressing the challenges associated with renewable energy integration, optimizing operational strategies, and advancing hydrogen storage technologies, these studies contribute to the creation of more efficient, reliable, and sustainable energy systems. The continued exploration and optimization of these systems are essential for realizing the full potential of hydrogen as a cornerstone of future energy landscapes.

6.2 Energy combination and management

The combination and management of diverse energy sources, particularly the integration of hydrogen storage with renewable energy systems, are pivotal for achieving a sustainable, efficient, and reliable energy supply. This section



(a) (b)

Fig. 5. (a) Schematic of a H_2–O_2 UR-PEMFC system, showing ideally a single cell as a power converter (Guarnieri et al., 2015). (b) Scheme of fluid mass transport occurring at flow channel and diffusion layer in the negative electrode, with convective (in BP) and diffusive (in DL) hydrogen flows, respectively in FC-mode operation (in EL-mode flow arrows reverse) (Guarnieri et al., 2015).

reviews key advancements in the field, emphasizing the role of hydrogen in enhancing the flexibility and sustainability of energy systems.

Parra et al. (2014) present a groundbreaking model that integrates photovoltaic generation, batteries, and hydrogen storage to bolster energy self-sufficiency and reliability in urban buildings. This comprehensive approach demonstrates the viability of combining various storage technologies for effective energy management, setting a precedent for future energy systems.

Teng et al. (2019) further the discussion with the development of a multi-energy storage system model based on electricity-hydrogen coupling. Their work illustrates the potential of hybrid energy storage systems to stabilize energy grids and increase renewable energy utilization, showcasing the flexibility provided by integrating hydrogen storage.

Tan et al. (2021) discuss an integrated energy system that combines hydrogen with natural gas, aiming to reduce carbon emissions and enhance the flexibility of the energy system. This approach highlights the potential for hydrogen to act as a bridge between renewable energy sources and traditional energy systems, facilitating a smoother transition to low-carbon energy solutions.

Wu et al. (2021) conduct a risk assessment for a wind-photovoltaic-hydrogen system, emphasizing the critical role of hydrogen storage in supporting sustainable energy transitions. Their work underlines the importance of comprehensive energy management strategies that incorporate hydrogen storage to ensure the resilience and sustainability of renewable energy systems.

The integration of hydrogen storage with renewable energy sources represents a significant stride toward the development of sustainable, efficient, and flexible energy systems. The studies highlighted in this section underscore the diverse approaches to energy combination and management, demonstrating the essential role of hydrogen in facilitating the widespread adoption of renewable energy. By leveraging the unique properties of hydrogen storage alongside other energy storage technologies, we can enhance the efficiency, reliability, and sustainability of future energy systems.

6.3 Techno-eco-economic analyses

Techno-eco-economic analyses provide a comprehensive framework for evaluating the viability and sustainability of hydrogen storage technologies within the context of global energy systems. These analyses integrate technical performance, economic feasibility, and environmental impact assessments to inform policy, investment, and research directions. This section reviews key contributions to the techno-eco-economic evaluation of hydrogen storage systems, highlighting their role in advancing sustainable energy solutions.

Garcia-Torres and Bordons (2015) emphasize the economic operation optimization of hydrogen-based renewable energy systems, particularly within smart cities. By considering the rules of the electricity market, their analysis seeks to maximize both economic benefits and sustainability, offering insights into the strategic deployment of hydrogen technologies in urban settings.

Eypasch et al. (2017) introduce a model-based techno-economic evaluation for an electrolyzer-based hydrogen storage system tailored to residential applications, as shown in Fig. 6(c). This study highlights the economic viability and integration potential of hydrogen storage with renewable energy sources, providing a pathway toward decentralized energy solutions.

Arsalis et al. (2018) focus on the thermoeconomic modeling of an autonomous zero-emission hydrogen-based power supply system. Their work showcases the system's potential to offer sustainable energy solutions, emphasizing the importance of integrating economic considerations in the design and optimization of hydrogen storage systems.

Jin et al. (2020) present a simulation study on a hydrogen-heating-power polygeneration system driven by supercritical water gasification, can be seen in Fig. 6(d). This approach underlines the system's efficiency in energy utilization and its potential for seamless integration with renewable energy sources, highlighting the economic and environmental benefits of polygeneration systems.

Izadi et al. (2022) conduct a transient simulation and techno-economic assessment of an off-grid hybrid renewable energy system incorporating hydrogen storage. Their findings demonstrate the system's potential for providing cost-effective and reliable energy supply, underscoring the importance of comprehensive evaluations in the development of hybrid energy systems.

The techno-eco-economic analyses discussed in this section are pivotal for understanding the multifaceted implications of hydrogen storage technologies. By balancing technical performance with economic feasibility and environmental considerations, these studies contribute to a holistic understanding of hydrogen's role in the energy transition. The ongoing research and evaluation efforts in this area are essential for identifying sustainable, economically viable, and technically robust hydrogen storage solutions that can support the global shift toward renewable energy.

7. Thermodynamics and kinetics

7.1 Heat and mass interactions

The efficiency of hydrogen storage systems is intricately tied to the dynamics of heat and mass interactions within these systems. This section delves into the significant contributions made towards understanding and optimizing these interactions, particularly in metal hydride and liquid organic hydrogen carriers.

Raju et al. (2019) introduce a comprehensive thermal modeling approach for intermetallic hydrides, offering a robust design methodology to enhance the efficiency of metal hydride hydrogen storage systems. Their work lays the groundwork for improving system design through detailed thermal analysis.

Chibani et al. (2020) explore heat and mass transfer processes during hydrogen storage in metal hydrides, contributing significantly to the optimization of hybrid energy storage systems, illustrated in Fig. 7(a). By integrating hydrogen storage with renewable energy sources, their research highlights the potential for improved system efficiency through optimized heat and mass transfer.

Valizadeh et al. (2016) simulate heat and mass transfer in a metal hydride hydrogen storage system, thereby improving the understanding of the storage mechanisms and enhancing system efficiency, displayed in Fig. 7(b). This simulation work is pivotal in identifying key factors that influence heat and mass interactions within the system.

Heublein et al. (2020) examine hydrogen storage using liquid organic carriers, highlighting the technology's potential for efficient and reversible hydrogen storage. Their work underscores the importance of understanding heat and mass transfer processes in the development of advanced hydrogen storage solutions.

Anbarasu et al. (2014) and Wang et al. (2020) focus on optimizing composite thermal insulation systems for liquid hydrogen storage tanks and conducting numerical studies on heat and mass transfer in metal hydride systems. These studies aim to enhance the safety and efficiency of cryogenic and metal hydride hydrogen storage by improving thermal insulation and optimizing performance.

The advancements in understanding and optimizing heat and mass interactions within hydrogen storage systems underscore the critical role of thermal management in achieving high efficiency and reliability. Through comprehensive modeling, simulation, and experimental investigations, researchers are paving the way for the development of more efficient, safe, and economically viable hydrogen storage solutions. The continuous exploration of heat and mass transfer processes is essential for the innovation and optimization of hydrogen storage technologies, ensuring their successful integration into the global energy system.

7.2 Thermo-physical and chemical energy storage

Thermo-physical and chemical processes play a vital role in the development of efficient and sustainable hydrogen storage solutions. This section explores the advancements in these areas, highlighting their potential to revolutionize hydrogen storage and release mechanisms.

Hamayun et al. (2019) explore the integration of hydrogenation-dehydrogenation processes, contributing significantly to the development of efficient hydrogen storage and release systems. Their work emphasizes the potential for chemical reactions to enhance storage density and reversibility, marking a pivotal advancement in chemical hydrogen storage technologies.

Ng et al. (2022) investigate the modeling of interfacial tension in hydrogen-based systems, underlining the importance of understanding these properties for developing efficient hydrogen storage technologies, displayed in Fig. 7(c). This study highlights the role of physical interactions in optimizing storage conditions and enhancing system performance.

Zehra et al. (2022) introduce a fuzzy-barrier sliding mode control for electric vehicles equipped with hydrogen storage, aiming to enhance vehicle stability and energy efficiency. This innovative approach underscores the integration of hydrogen storage with vehicle dynamics, contributing to the development of more efficient and reliable hydrogen-powered vehicles.

Kuroki et al. (2021) model the thermodynamics of hydrogen fueling processes, providing insights into the optimization of fueling stations for high-pressure hydrogen storage. Their work is crucial for improving the efficiency and safety of hydrogen refueling, facilitating the broader adoption of hydrogen as a fuel.

Pinto et al. (2021) model the phase equilibrium of hydrogen and natural gas mixtures using the e-PPC-SAFT equation of state, contributing to the optimization of gas storage and transport processes. This study emphasizes the potential for hydrogen to be integrated into existing natural gas infrastructures, enhancing the flexibility and sustainability of energy systems.

López-Chávez et al. (2020) investigate the thermodynamic conditions for hydrogen sulfide and carbon monoxide absorption in ionic liquids, offering insights into purification pro-

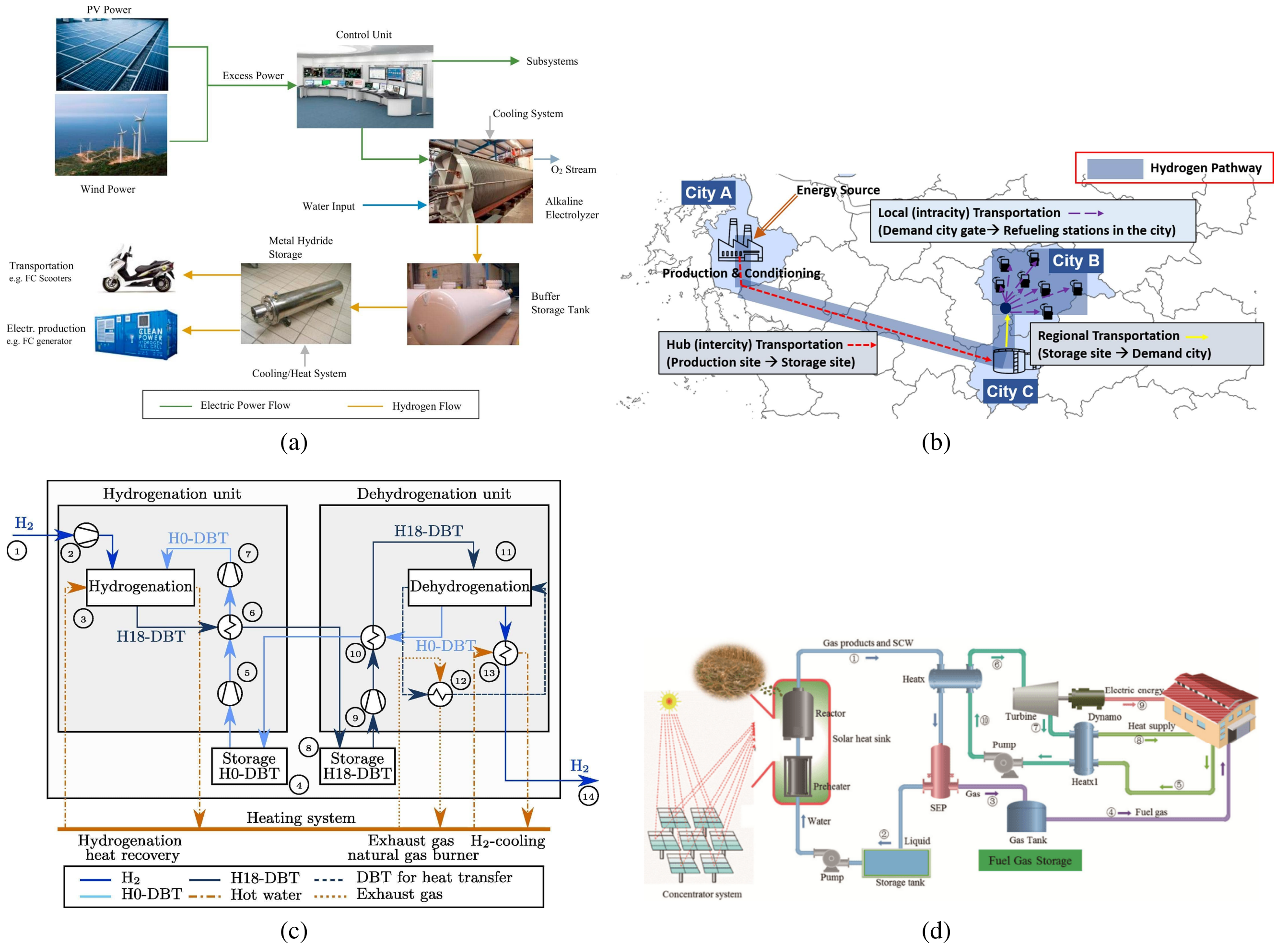


Fig. 6. (a) Description of the hydrogen production-storage system (Kavadias et al., 2018). (b) Concept of hydrogen pathways in a supply chain (Seo et al., 2020). (c) Liquid Organic Hydrogen Carrier system overview (Eypasch et al., 2017). (d) Schematic diagram of gas-heat-power poly-generation energy storage system (Jin et al., 2020).

cesses relevant to hydrogen production. Their work highlights the importance of clean hydrogen production for ensuring the sustainability of hydrogen energy systems.

The integration of thermo-physical and chemical processes in hydrogen storage technologies represents a significant stride toward achieving efficient, safe, and sustainable energy storage solutions. Through the contributions outlined in this section, the field is advancing towards innovative storage mechanisms that promise higher densities, improved reversibility, and integration with renewable energy sources. The ongoing research and development in thermo-physical and chemical energy storage are vital for unlocking the full potential of hydrogen as a key component of the future energy landscape.

7.3 Statistical thermophysics

Statistical thermophysics plays a crucial role in elucidating the fundamental mechanisms underlying hydrogen storage in various materials, including MOFs, nanoporous materials, and nanostructured materials. By leveraging advanced computational methods, researchers have gained profound insights into the thermodynamic and kinetic aspects of hydrogen storage, paving the way for the development of more efficient storage solutions.

Abdellaoui et al. (2020) utilize first-principle calculations and kinetic Monte Carlo simulations to examine hydrogen storage in nanoporous materials, demonstrating how material properties significantly impact storage efficiency, illustrated in Fig. 7(d). This study underscores the importance of material structure and composition in optimizing hydrogen storage capacities.

Yu et al. (2020) explore the hydrogen storage capabilities of MOF-5 through grand canonical Monte Carlo simulations, highlighting the potential of MOFs as highly efficient hydrogen storage materials due to their large surface areas and tunable porosity. This research exemplifies the power of computational simulations in predicting and enhancing the performance of hydrogen storage materials.

Mahdizadeh et al. (2014) investigate the storage capabilities of silicon carbon and silicon carbide nanotubes, emphasizing the influence of tube diameter on storage efficiency. Their work, using grand canonical Monte Carlo simulations, contributes to the understanding of nanostructured materials' role in hydrogen storage.

Sunnardianto et al. (2021) assess the hydrogen storage potential of defective graphene, employing a combination of density functional theory and grand canonical Monte Carlo simulations to improve storage capacities. This study reveals how defects within the graphene structure can enhance hydrogen adsorption, offering pathways to tailor materials for increased storage efficiency.

Caviedes et al. (2022) apply grand canonical Monte Carlo simulations to study hydrogen adsorption in nanoporous materials, showcasing the accuracy of computational methods in predicting storage capacities. This research highlights the critical role of statistical thermophysics in advancing our understanding of hydrogen storage mechanisms and optimizing material designs for enhanced storage performance.

The application of statistical thermophysics to hydrogen storage research has significantly advanced our understanding of the complex interactions governing hydrogen adsorption and desorption. Through the integration of computational simulations and theoretical models, researchers have identified key factors that influence the efficiency and capacity of hydrogen storage materials. These insights are instrumental in guiding the development of next-generation hydrogen storage solutions that combine high storage capacities with favorable thermodynamic properties, contributing to the broader adoption of hydrogen as a clean and sustainable energy carrier.

8. Molecular dynamics and simulations

8.1 Hydrogen storage capacity and mechanisms

Understanding the capacity and mechanisms of hydrogen storage from molecule scale is pivotal for advancing hydrogen energy systems. This section synthesizes key findings from recent research, offering molecular dynamics insights into the development of efficient and reliable storage solutions.

Kolesnik et al. (2018) introduce a new hydride reorientation model for magnesium-based storage systems, enhancing the understanding of metal hydride storage mechanisms. This work is instrumental in optimizing the hydrogen absorption and desorption processes, crucial for metal hydride storage systems.

Kim et al. (2017) describe a one-dimensional numerical model focusing on thermal and mass transfer processes in metal hydrides, aiming to optimize storage system performance. Their work highlights the importance of integrated thermal management strategies for improving hydrogen storage efficiency.

Neves et al. (2021) discuss the Lithium-Boron Reactive Hydride Composite System for hydrogen storage, emphasizing its potential for efficient energy storage and release. This innovative composite system showcases the synergy between different materials to enhance hydrogen storage capacity and reversibility.

Jaiswal et al. (2022) address reversible hydrogen storage in metal hydrides from a materials science perspective, focusing on enhancing storage efficiencies through material modification and optimization. Their research underscores the critical role of material engineering in advancing hydrogen storage technologies.

Yang et al. (2023a, 2023b) conducted a series of molecular dynamics simulations to clarify the interfacial properties of the hydrogen with water and other gas mixture with the presence of different type of rocks at various temperatures and pressures, revealing the interfacial tension variation mechanisms, displayed in Fig. 8(a).

The advancements in hydrogen storage capacity and mechanisms from molecule perspective, as discussed in this section, underscore the multifaceted approach required to develop efficient hydrogen storage solutions. These insights are crucial for the ongoing development of hydrogen storage technologies, aiming to maximize storage capacity, efficiency, and system reliability. As research progresses, the integration of material science, thermodynamics, and system design will continue to play a vital role in overcoming the challenges associated with hydrogen storage.

8.2 Functionalization and enhancement strategies

In the quest for optimal hydrogen storage solutions, functionalization and enhancement strategies play pivotal roles, leveraging molecular simulations to unravel the complexities of material behavior and interaction with hydrogen. This section explores cutting-edge research that employs these strategies to significantly enhance hydrogen storage capacities and mechanisms.

Kag et al. (2021) and Chakraborty et al. (2022a) examine the potential of graphene and triazine-based frameworks, respectively, for hydrogen storage, utilizing strain, defect engineering, and metal decoration to increase storage capacities. Their findings illuminate the path toward designing materials with tailored properties for superior hydrogen adsorption.

Krylova et al. (2020) focus on the unique properties of crumpled graphene, emphasizing its enhanced surface area and its implications for increased hydrogen storage capacity, can be seen in Fig. 8(b). This underscores the importance of material morphology in designing effective storage media.

Simagina et al. (2017) investigate ammonia borane's hydrogen storage capabilities, highlighting its role as a solid hydrogen carrier with favorable dehydrogenation properties. This research points to the chemical routes as viable paths for hydrogen storage enhancement.

Gebhardt et al. (2014) explore metal oxide model clusters for hydrogen storage, demonstrating how low-coordinated sites can significantly improve hydrogen adsorption. This study showcases the effectiveness of surface functionalization in optimizing material interactions with hydrogen.

Further contributions by Tokarev et al. (2015) and Mane et al. (2022b) illustrate how boron substitution in graphene and decoration with alkali metals can lead to substantial increases in hydrogen storage capacities. These modifications enhance material-hydrogen interactions, paving the way for advanced storage solutions.

The innovative functionalization and enhancement strategies highlighted in this section, facilitated by molecular simulations, mark a significant advancement in hydrogen storage

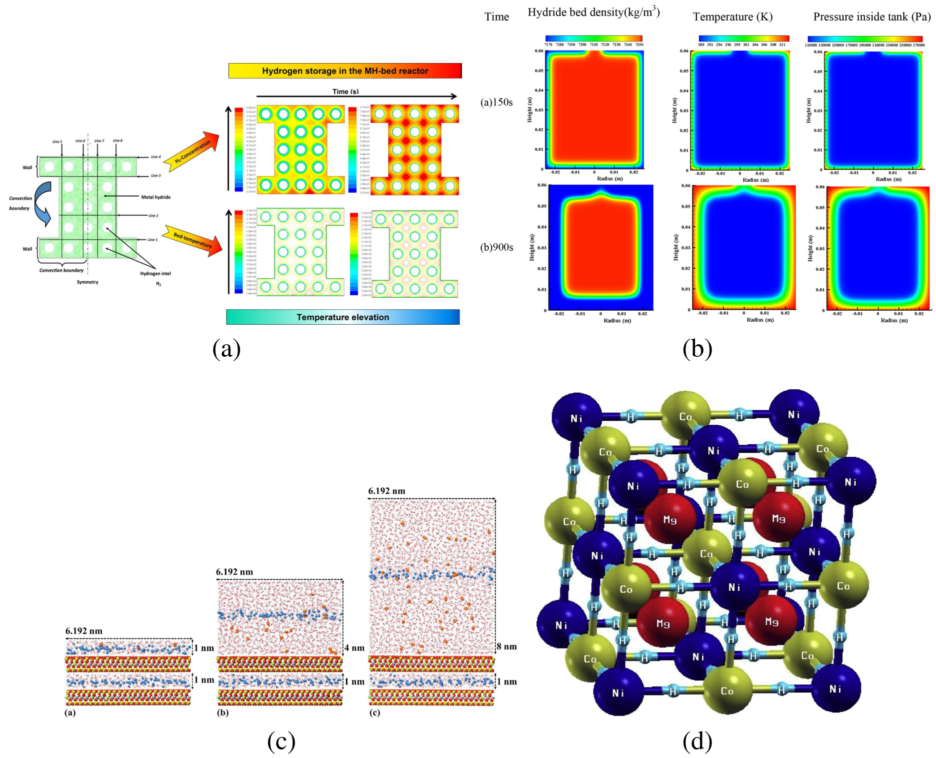


Fig. 7. (a) Graphical abstract of Heat and mass transfer during the storage of hydrogen in LaNi5-based metal hydride: 2D simulation results for a large scale, multi-pipes fixed-bed reactor (Chibani et al., 2020). (b) Contours of metal hydride bed density, bed temperature and pressure inside tank. Tf = 313 K and *Pout* = 0.1 MPa. a) t = 150 s b) t = 900 s (Valizadeh et al., 2016). (c) Snapshots of the three different supercell structures of the Na-montmorillonite slab with interlayer space of a) 1 nm, b) 4 nm, and c) 8 nm in contact with water containing hydrogen. Color hint: Si, yellow; Al, gray; Mg, green; O, red; Na, blue; and H, white. Note that, for better clarity, water molecules are shown smaller, and interlayer hydrogen molecules are demonstrated in orange (Ng et al., 2022). (d) Supercell presented $MgCo_0 \cdot 5Ni_0 \cdot 5H_3$; Magnesium atoms are in red, Cobalt atom in yellow, Nickel atom in blue dark and hydrogen atoms in blue (Abdellaoui et al., 2020).

technology. By tailoring material properties through strategic modifications, researchers have unlocked new potentials in hydrogen storage capacities and efficiencies. These strategies, ranging from defect engineering to chemical functionalization, are instrumental in overcoming the limitations of traditional hydrogen storage materials, offering promising avenues for the development of next-generation hydrogen storage systems.

9. Machine learning and big data

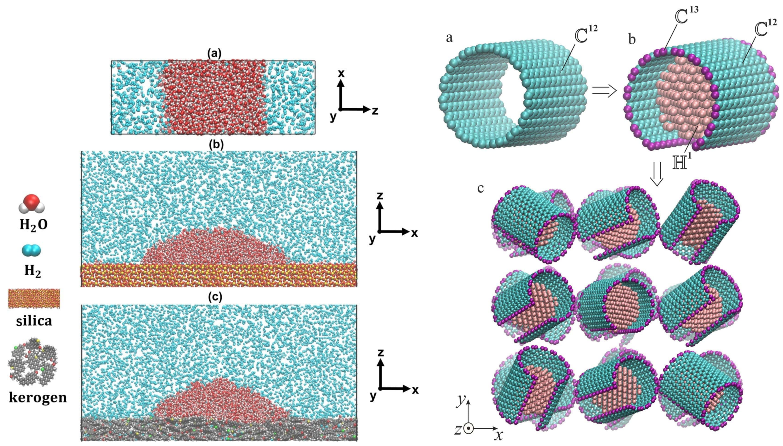
Machine learning and big data analytics offer groundbreaking approaches to addressing the challenges of hydrogen storage. Through predictive modeling, optimization algorithms, and the analysis of vast datasets, these technologies enable the rapid exploration of material properties, storage mechanisms, and system designs (Song et al., 2022; Du et al., 2023a, 2023b; Xie et al., 2023a, 2023b). As the field of hydrogen storage progresses, the integration of machine learning and big data analytics will continue to play a crucial role in unlocking new potentials, enhancing storage capacities, and advancing towards a sustainable energy future.

Zhang et al. (2024) developed a deep learning algorithm using a thermodynamics-informed neural network to perform accurate, robust, and fast phase equilibrium calculations for realistic fluid mixtures of natural hydrogen, which accelerated the calculations for 20 times compared to direct thermodynamics simulation, can be seen in Fig. 9(a).

Alaiz-Moretón et al. (2019) pioneer the use of machine learning techniques to predict hydrogen storage capacities, demonstrating the potential of ML algorithms to uncover complex patterns and relationships in storage data, as shown in Fig. 9(b). This approach marks a significant advancement in optimizing storage systems, reducing the time and resources required for empirical testing.

Bobbitt and Snurr (2019) have pioneered the application of molecular modeling and machine learning to predict hydrogen storage performance in MOFs, setting a precedent for the use of advanced computational methods in material science, illustrated in Fig. 9(c). Their approach not only enhances the storage capacities but also streamlines the material design process for targeted applications.

Li et al. (2014) apply big data analytics to simulate and analyze experimental data on hydrogen storage, showcasing the importance of integrating experimental and computational research. This synergy between big data and experimental validation enhances the reliability and accuracy of predictive models, facilitating a deeper understanding of storage mecha-



(a) (b)

Fig. 8. (a) Equilibrium snapshots of the a) H_2+H_2O system, b) H_2+H_2O+silica system, and c) H_2+H_2O+kerogen system at 373 K and 80 MPa. Color code for H_2O: O, red; H, white. Color code for H_2: H, cyan. Color code for silica: Si, yellow; O, red; H, white. Color code for kerogen: C, grey; O, red; N, yellow; S, green; H, white (Yang et al., 2023a, 2023b). (b) Schematic of how the initial structure of crumpled graphene is obtained: carbon nanotube (15, 15) 2.5 nm long a) graphene flake with hydrogen atoms inside b) crumpled graphene, made of randomly oriented graphene flakes, repeated along three x, y and z-coordinates c) Hydrogen atoms H_1 are pink, carbon atoms C_{12} are turquoise, and edge carbon atoms C_{13} with higher molar mass are purple (Krylova et al., 2020).

nisms and material behaviors.

These studies illustrate the transformative potential of machine learning and big data analytics in hydrogen storage research. By harnessing these technologies, researchers can accelerate the development of efficient, high-capacity storage solutions, paving the way for the broader adoption of hydrogen as a sustainable energy carrier.

10. Challenges and future research topics

The exploration of hydrogen storage modeling and simulations has revealed significant advancements across various storage methods, including UHS, materials science, system integration, and the application of advanced computational techniques. These developments underscore both progress and potential areas for future exploration, highlighting specific challenges and suggesting directions for future research.

10.1 Challenges

1) UHS faces challenges in identifying suitable geological formations that ensure safety and environmental protection while maintaining high storage efficiency. Addressing the long-term effects of hydrogen on rock integrity and the potential for gas leakage are critical for the advancement of UHS technologies.
2) Solid Material Hydrogen Storage struggles with finding materials that offer high hydrogen storage capacity at practical operating temperatures and pressures. The kinetics of hydrogen absorption and desorption, material stability over repeated cycles, and the cost of storage materials remain significant challenges.
3) High-Pressure Compression Storage must overcome issues related to the materials used for storage tanks, including weight, cost, and safety under extreme pressure conditions. Developing lightweight, durable, and cost-effective materials that can withstand high pressures is essential.
4) Fuel Cell On-Board Storage faces the dual challenge of maximizing energy density while minimizing weight and volume. Achieving rapid refueling times and ensuring long-term stability and safety under the varying conditions of vehicle operation are ongoing challenges.
5) Hybrid Energy Systems incorporating hydrogen storage need to address the integration of diverse energy sources and storage technologies to ensure seamless operation. Optimizing these systems for efficiency, reliability, and cost-effectiveness in a fluctuating energy market poses a complex challenge.
6) Thermodynamics in hydrogen storage systems requires a deeper understanding of heat and mass transfer processes, especially in solid-state and liquid hydrogen storage, to enhance system efficiency and performance.
7) Molecular Dynamics studies of hydrogen storage materials face challenges in accurately predicting material behavior and hydrogen interactions at the atomic and molecular levels, necessitating more sophisticated models and computational methods.
8) Machine Learning applications in hydrogen storage research are challenged by the need for large, high-quality datasets for training models and the complexity of integrating ML predictions with empirical research findings for real-world applications.

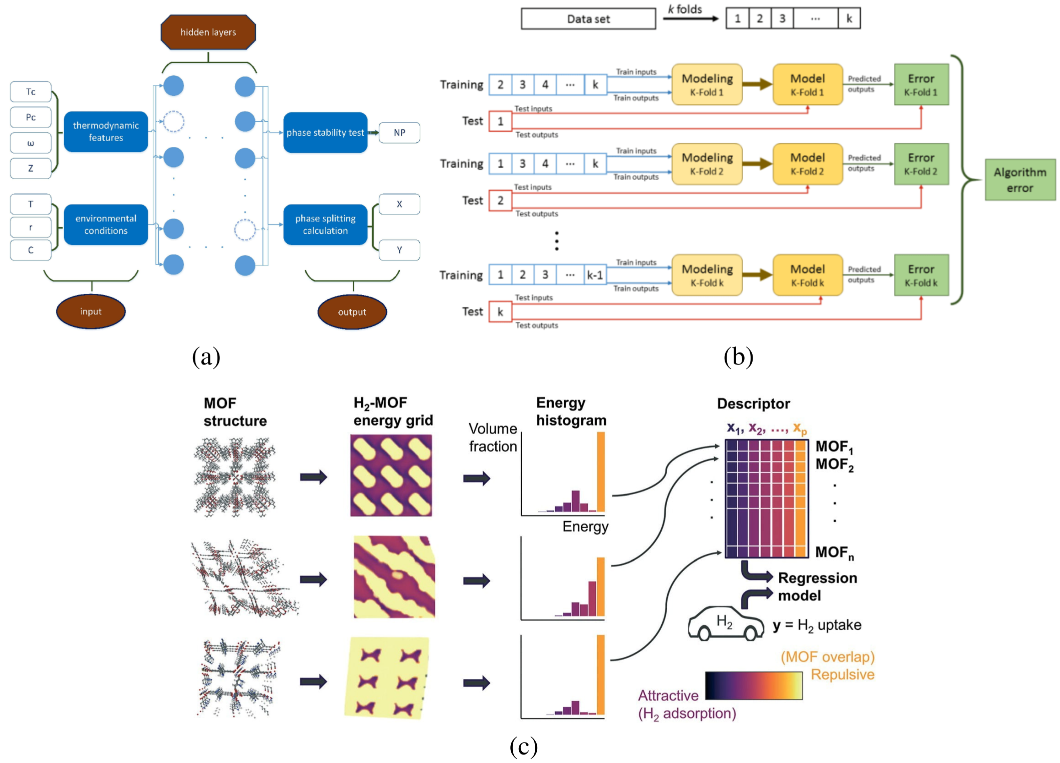


Fig. 9. (a) Schematic of the thermodynamics-informed neural network architecture (Zhang et al., 2024). (b) K-Fold training and test data selection (Alaiz-Moretón et al., 2019). (c) Schematic of machine learning workflow. For each MOF, the 3D potential energy surface is calculated using a H_2 probe molecule on a grid. The distribution of energies of the grid are represented as an energy histogram, and each bin of the histograms is an input into the LASSO model (Bobbitt and Snurr, 2019).

10.2 Future research topics

1) Underground Hydrogen Storage UHS research should focus on advanced geological surveys and modeling to identify optimal storage formations, along with studies on the long-term effects of hydrogen storage on geological structures. Developing monitoring and mitigation strategies for potential environmental impacts will also be crucial.
2) Solid Material Hydrogen Storage future topics include the discovery and development of novel materials with enhanced hydrogen storage capacities and favorable thermodynamics. Research should also explore the improvement of kinetics for hydrogen absorption/desorption and the lifecycle stability of storage materials.
3) High-Pressure Compression Storage research should aim at the development of new composite materials for tanks that offer improved strength-to-weight ratios and resistance to hydrogen embrittlement. Innovations in tank design to reduce costs and enhance safety are also needed.
4) Fuel Cell On-Board Storage should investigate compact, lightweight storage solutions that allow for quick refueling and high energy density. Developing materials and systems that can operate effectively over a wide range of temperatures and pressures is essential for vehicle applications.
5) Hybrid Energy Systems incorporating hydrogen storage will benefit from research into system integration, focusing on optimizing the balance between renewable energy generation, hydrogen storage, and energy consumption patterns. Advanced control systems and algorithms for managing these integrated systems are key areas for future exploration.
6) Thermodynamics research should delve into enhancing the efficiency of heat and mass transfer in hydrogen storage systems, particularly for solid-state and liquid storage methods. Developing innovative thermal management strategies to control system temperatures during charging and discharging phases is crucial.
7) Molecular Dynamics studies should aim to refine computational models for better prediction of material properties and hydrogen interactions. This includes leveraging quantum mechanics simulations and high-performance computing resources to explore the potential of novel hydrogen storage materials.
8) Machine Learning in hydrogen storage research should focus on generating and utilizing extensive datasets to train models capable of predicting material behaviors and system performances. Integrating machine learning predictions with experimental research to accelerate the development of efficient hydrogen storage solutions is a promising area for future research.

11. Conclusions

The review of hydrogen storage modeling and simulations highlights the dynamic interplay between technological advancements and the challenges that remain. Through detailed exploration of underground storage, solid-state materials, high-pressure systems, and the integration of machine learning and big data analytics, this review underscores the significant strides made towards efficient, safe, and economically viable hydrogen storage solutions. However, the journey towards optimizing hydrogen storage is far from complete. The outlined challenges and future research topics provide a roadmap for researchers, indicating critical areas where innovation and investigation can contribute to the realization of hydrogen's full potential as a cornerstone of the sustainable energy landscape. As we move forward, the continued synergy between experimental research and computational modeling will be pivotal in overcoming current limitations and unlocking new opportunities in hydrogen storage technology.

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Conflict of interest

The authors declare no competing interest.

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