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REVIEW PAPER

Scientometric analysis of computational calculations on hydrogen adsorption

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ABSTRACT

The rapid industrialization has driven economic growth and population increase, but it has also led to significant environmental issues and energy shortages. To effectively tackle these challenges and move towards a carbon-neutral energy framework, it is crucial to examine clean energy options and diminish reliance on fossil fuels. Among these alternatives, hydrogen stands out as a leading candidate due to its energy density and environmental affinity, being both abundant and renewable. This study delivers a thorough overview of the yearly scientific activities concerning hydrogen adsorption and storage, segmented by country and authorship. The study aims to evaluate the evolution of this field, its thematic shifts, and the dynamics of worldwide collaboration. The present research was conducted in the databases Web of Science and Scopus from 2000 to 2022, using a pre-determined set of keywords related to hydrogen adsorption, storage, and density functional theory. The retrieved data were analysed with the bibliometrix package in RStudio to evaluate publication trends, research evolution across three distinct periods and global collaboration networks. The current study focused on identifying a total of 2,183 documents, which were later evaluated and organized according to their relevance to the topic of hydrogen storage. In the present work, 881 articles were assessed for eligibility, identifying 60 key studies through degree and PageRank metrics, the evolution of research is delved into throughout three key stages. The three distinct periods identified were: the initial stage (2000-2008) which was marked by fundamental work on ionic liquids and hydrogen storage. The intermediate stage (2009-2015) witnesses an increase in scientific production, addressing fundamental principles and methodologies with a focus on metal-organic frameworks. The current stage (2016-2022) is characterized by optimal productivity, highlighting innovative investigations into nanotubes and electrocatalysts that facilitate the effective generation of hydrogen. The study explores global collaboration networks between countries and identifies influential authors and leading journals in the field. By the identification of the key trends, this study highlights the emergence of novel materials and technologies that are reshaping the hydrogen storage landscape. Such progress points to prospective directions for future research and innovation, thereby playing a crucial role in the advancement of sustainable energy solutions. This bibliometric study yields significant insights into the evolving trends, contributions, and collaborative dynamics that are defining the field of hydrogen adsorption and storage research landscape.

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INTRODUCTION

Phenomena as global warming is direct effect of the use of fossil fuels, since they emit large amounts of pollutant and greenhouse effect gases as carbon dioxide (CO_2), sulfur dioxide (SO_2), and nitrogen dioxide (NO_2) among other pollutants. The environmental risks associated with fossil fuels necessitate their eventual discontinuation, prompting a rapid shift towards renewable energy solutions (Fatima, 2021; Shiva Kumar and Himabindu, 2019). In addition to the aforementioned, it is necessary to find/implement high-density, sustainable, and scalable energy sources as alternative to the increase of the energy demand, and to mitigate the environmental impact of fossil-based energy sources. The rising interest in hydrogen (H_2) as a sustainable and clean energy solution stems from the fact that it produces only water as a by-product. H_2 generated from renewable energy sources can be a potential long-term vector of clean energy (Kammen and Sunter, 2016; Kazim and Veziroglu, 2001). There are different sources for H_2 generation including biomass, fossil fuels and water electrolysis (Megia *et al.*, 2021; Zhang *et al.*, 2021). The H_2 production for water splitting through electrolysis have been considered a possible renewable energy source, since it does not produce pollutants gases in the air and, therefore, this method becomes a potential to solve energy and environmental dilemmas in the global production of fuel (Guo *et al*., 2021; Hosseini *et al*., 2015). Likewise, in a similar vein, H_2 molecules can serve as a source of power for fuel cells and electricity generation. A vital consideration in the electricity-H_2-electricity conversion process is the necessity of integrating a storage phase within the hydrogen production and management system to ensure efficient use (Akarsu and Serdar Genç, 2022; Dematteis *et al*., 2021; Otsuka *et al*., 2003). However, current H_2 storage is usually produced at low temperature and at high pressure, being those subjects some of the problems to be solved for the implementation of the storage stage (Meng *et al*., 2023; Zhang *et al*., 2020). Addressing this challenge requires the storage of H_2 in an adsorbent material characterized by high porosity, as the efficiency of H_2 adsorption on its surfaces or within its structure is largely dependent on the surface properties (Singh *et al*., 2020; Wang *et al*., 2009; Yamashita *et al*., 2015). To reach H_2 storage at room temperature, it is needed that the adsorbent material has an adsorption energy ranging from 0.2 to – 0.6 electron volt (eV) (Choudhary *et al*., 2016; Maggio *et al*., 2019). In the case of physisorption, H_2 molecules interact with the material through long range vander Waals (vdW) forces, which is usual in materials with organometallic structures, zeolites and carbon-based materials, which allows H_2 to be easily absorbed and desorbed due to its low adsorption energy but having a low storage capacity at room temperature (Bénard and Chahine, 2007; Mohan *et al*., 2019). In the alternative scenario of chemisorption, individual H_2 molecules are bonded to the material via a covalent bond characterized by a significantly high adsorption energy. This occurs in materials such as metal hydrides that have a high capacity of H_2 storage at room temperature, even though they have slow adsorption and desorption of H_2 under very specific conditions (Bérubé *et al*., 2007; Feng *et al*., 2017). An essential challenge today is to advance the material characteristics suitable for H_2 storage under application conditions. This has resulted in the increase of theoretical studies in which various computational methodologies as density functional theory (DFT) have been employed, as several of these materials used in H_2 storage are difficult to synthesize (Carraro *et al.*, 2019; Amaya-Roncancio *et al.*, 2022). However, by utilizing computational calculations, challenges related to formation energy, energy diffusion barriers, and thermal stability can be resolved, enabling the development of suitable materials for H_2 applications (Guo and Wang, 2018a, 2018b; Sosa *et al*., 2023). One way to compile the state of the art of the aforementioned (materials for H_2 adsorption and storage) is to carry out a bibliometric analysis (BA). Quantitative analysis of published papers is achieved through bibliometric methods, which provide a standardized set of indicators. In this way, they assess the impact on the future of a field by tracking the citations of published materials (Tu *et al*., 2021). A BA is an analytical approach that identifies both existing and historical research trends in a given area of study. It utilizes data from academic literature and databases to create new research findings and to provide a broad overview of substantial amounts of information from scientific and scholarly works (Ellegaard and Wallin, 2015; Md Khudzari *et al*., 2018; Maphosa and Maphosa, 2022). Furthermore, bibliometric analysis has been used as a qualitative and quantitative method in the evaluation of

scientific literature in different disciplines (Ellegaard and Wallin, 2015; van Nunen *et al*., 2018). A BA can be classified into two key types: 1) assessments of productivity, which involve elements such as countries, authors, journals, publication years, and academic disciplines, and 2) literature reference and citation analyses, which concentrate on the works and authors that are cited (Hood and Wilson, 2001; Huang *et al*., 2024). In addition, authorship collaboration, word cloud, and scientific mapping networks are often used (Cobo *et al*., 2011; Molontay and Nagy, 2021; Danya *et al*., 2024). Understanding the evolution of the computational studies related with H_2 storage and H_2 production is a key aspect, not only in the comprehension of materials science, but also in the field of the evolution of the H_2 technology and the search for the explanation of the molecular mechanisms involved in H_2 processes. While many experimental and computational investigations have focused on the fundamental interactions of H_2, it is vital to achieve a complete understanding of its structural stability, saturation, energetic characteristics, and thermodynamic effects (Amaya-Roncancio *et al*., 2018, 2022). Therefore, molecular and computational studies related with H_2 should be revised in their several historical stages as an exercise of perspective, the historical evolution of the research related with H_2 can be handled under a scientometric review (Bhat *et al*., 2022; Śmiechowski, 2015). Considering the observations outlined, this study aims to perform a BA of scientific publications that concentrate on theoretical research advancements utilizing DFT for the purpose of production, adsorption, and storage. Understanding its fundamental aspects, contributing and promoting the development of environmental sustainability. In addition, a scientometric mapping was carried out in three states (2000-2008, 2009-2015 and 2016-2022), in which global collaboration networks between countries were also added, with which the most influential authors and the most outstanding journals in this area were identified. The current study was carried out in Colombia by BA tools in the year 2023 as the necessity of understanding the evolution of the H_2 storage technologies and computational calculations.

MATERIALS AND METHODS

In order to comprehend the scientific landscape of the research field, a scientometric analysis was performed in 2022 utilizing Web of Science (WoS) and Scopus databases, covering the period from 2000 to 2022. The search was conducted to identify relevant articles on H_2 adsorption and storage using Eq. 1 (He *et al*., 2019):

TITLE (hydrogen AND adsorption) OR TITLE (hydrogen AND storage) AND TITLE-ABS-KEY (dft) AND PUBYEAR> 2000, AND PUBYEAR <2022 (1)

It is worth noting that, to implement these search parameters, the databases needed to be combined and evaluated through exploratory data analysis (EDA) by the use of scientometric tools such as Bibliometrix. This technique allowed for the structured compilation of relevant data and references, delivering an in-depth overview of contemporary studies and increasing the efficiency of the BA concerning the variable under analysis. Table 1 shows the parameters employed in the study. For instance, specific search terms were applied to the

Table 1: Search parameters

Databases	Web of Science	Scopus
Consultation period (in year)	2002-2022	2002-2022
Consultation date	April 26th, 2022	April 26th, 2022
Document type	Article, review, …	Article, review, …
Magazine type	All types	All types
Search fields	TITLE-ABS-KEY	TITLE-ABS-KEY
	TITLE (hydrogen AND adsorption)	TITLE (hydrogen AND adsorption)
	OR TITLE (hydrogen AND storage)	OR TITLE (hydrogen AND storage)
Search terms Eq. 1	AND TITLE-ABS-KEY (dft) AND	AND TITLE-ABS-KEY (dft) AND
	PUBYEAR > 2000 AND PUBYEAR <	PUBYEAR > 2000 AND PUBYEAR <
	2022	2022
Results	1104	1079
Total results	1396	

Table 2: PRISMA Statement Identification of studies via databases and registers

Section	Category	Description	Count
Identification	Records through database searching	Web of Science	1104
Identification		Scopus	1079
Identification	Identification of additional records by other sources	--	0
Identification	Duplicates removed	--	2183
Screening	Records screened	--	2183
Screening	Records excluded	--	1302
Eligibility	Full articles assessed for eligibility	--	881
Eligibility	Excluded full-text articles	Unrelated documents	22
Eligibility		Reviews excluded	53
Included	Studies included in qualitative synthesis		28
Included	Studies included in quantitative synthesis (meta-analysis)		60

title, to the abstract, and to the keywords to locate articles related to the academic's role as a researcher. A total of 1104 entries were obtained from the WoS, while Scopus provided 1079 entries. The data from these two databases were merged through the use of the 'bibliometrix' packages.

The preferred reporting items for systematic reviews and meta-analyses (PRISMA) flow proposed by Liberati *et al*. (2009), outlines the refinement process used to narrow down the documents, resulting in a highly relevant and suitable sample for the analysis presented in this article. The network consists of 881 scientific papers and 2962 connections, with 60 publications considered as relevant and identified based on its metrics. In total, 28 articles were manually selected that address H_2 adsorption, H_2 storage, and computational calculations. After eliminating duplicate entries, the remaining documents were assessed by two authors to filter out reviews and papers deemed irrelevant. In this line, 22 articles unrelated to the main subject and a total of 53 review papers were identified. The unrelated documents were excluded at this stage, as reviews, while summarizing existing knowledge, do not contribute new findings. Ultimately, this process resulted in a dataset containing 91087 coded articles. The subsequent section outlines the coding process. Additional details regarding the data analysis conducted in this study can be found in Table 2.

In the process of selecting references, emphasis was placed on manuscripts that clearly contained keywords such as "hydrogen," "storage," and "hydrogen production," thus guaranteeing their direct connection to the research focus. The chosen manuscript was required to contain a detailed methodology involving DFT and computational calculations, particularly those with high citation counts, indicating their impact and relevance in the field. In contrast, the exclusion criteria disqualified any manuscripts that were not significantly cited, lacked computational studies relevant to the molecular comprehension of H_2 storage, production, or adsorption, or were published in languages other than English.

RESULTS AND DISCUSSION

This session provides a comprehensive overview of the annual scientific output, including a breakdown by country, an analysis of authorship, and an in-depth examination of the leading journals.

Scientific production

The annual publication data from Scopus and WoS, as well as the total counts of publications and citations for each year, are presented in Fig. 1. To better understand the various phases connected to

the topic throughout the years, a three-part analysis was undertaken, highlighting critical factors of productivity and their respective citation metrics.

Stage 1: Initial development phase (2000 - 2008)

During the initial growth stage, which spanned from 2000 to 2008, a major breakthrough was the use of ionic liquids to improve the dehydrogenation of amine boranes. The exceptional attributes of these liquids were instrumental in optimizing the process. These liquids exhibit distinctive characteristics, including low vapor pressure, stability at elevated temperatures, and the capacity to dissolve a diverse array of compounds and gases. These characteristics provide a more inert reaction medium that stabilizes polar transition states, facilitating a more efficient release of H_2. This stage is highlighted by the influential paper by Bluhm *et al*. (2006), who indicated that ionic liquids offer advantage for ammonia borane systems based in chemical H_2 with storage usages temperatures between 85 and 95 degrees Celsius (°C), there is a marked enhancement in both the amount of hydrogen produced and the rate of its release during the dehydrogenation of ammonia borane. This improvement is observed in a 1-butyl-3-methylimidazolium chloride medium, as opposed to the corresponding reactions occurring in solid form. In the academic community, this article has had a notable impact by registering the maximum number of citations, with a total of 568 mentions in other documents. The key aspect is that the physicochemical properties of ionic liquids render them a compelling choice for H_2 storage applications. The speed of release of H_2, the operating temperature and the purity of H_2 are fundamental aspects that have generated research interest in the creation of improved ionic liquid compounds for the storage of this gas (Himmelberger *et al*., 2009; Ren *et al*., 2017; Stracke *et al*., 2007). In this sense, it has been reported that the ionic liquid methylguanidinium borohydride (N_3H_8C]C+BH_4) has a 9.0 weight percent (wt%) of release capacity of H_2 under conditions of catalisys (Doroodian *et al*., 2010). Reports indicate that the combination of the guanidinium cation with the octahydrotriborate anion leads to the formation of guanidinium octahydrotriborate, which possesses a H_2 storage capacity of 13.8 wt% (Chen *et al*., 2015). Another relevant study is the one carried out by Mpourmpakis *et al*., 2006, with 358 citations, in which they researched H_2 storage in silicon-carbon nanotubes (SiCNTs) using a multiscale theoretical approach. The results emphasize that DFT calculations demonstrated a rise in H_2 bonding energy relative to pure carbon nanotubes (CNTs). Furthermore, the classical Monte Carlo simulation reflected that SiCNTs nanotubes have a greater storage capacity, especially under low temperature and high-pressure conditions. This simulation illustrates the emergence and evolution of themes, which accounts for the limited output of articles. Nevertheless, a considerable number of citations (9548) is evident in subsequent research, indicating progress in the consolidation and recognition of this topic in the academic field. It is essential to recognize that the studies published at this point lay the groundwork for future research and academic endeavors focused on adsorption mechanisms, H_2 storage capacity and DFT calculations.

S*tage 2: Intermediate stage of development (2009 - 2015*)

The second stage reveals a marked increase in scientific production, significantly exceeding the growth seen in the first stage. Likewise, the research topic experienced a substantial advance in its level of maturity, establishing more robust foundations in terms of fundamental principles, methodologies and possible applicable adaptations of knowledge, thus promoting the evolve of future investigations in relation with the initial topic. This analysis is predicated on the observation that, in this period, certain years exhibit a markedly higher citation count compared to the number of publications, as shown in Fig. 1. This figure is approximately four times greater than the corresponding value observed in the first phase. In the second period of time, the stage 2, the work carried out by Han *et al. (*2009) stands out. This work has obtained around 514 citations. This manuscript provided a comprehensive review of theoretical research related to hydrogen storage in metal-organic frameworks (MOFs) and covalent organic frameworks (COFs). The significance of the in silico methodology is highlighted for its ability to deliver essential insights, including H_2 adsorption sites, storage capacity, and H_2 diffusion characteristics. The use of quantum mechanics is mentioned to calculate H_2 adsorption sites in MOFs and COFs, either by ab initio or DFT methods. The H_2 storage capacity in

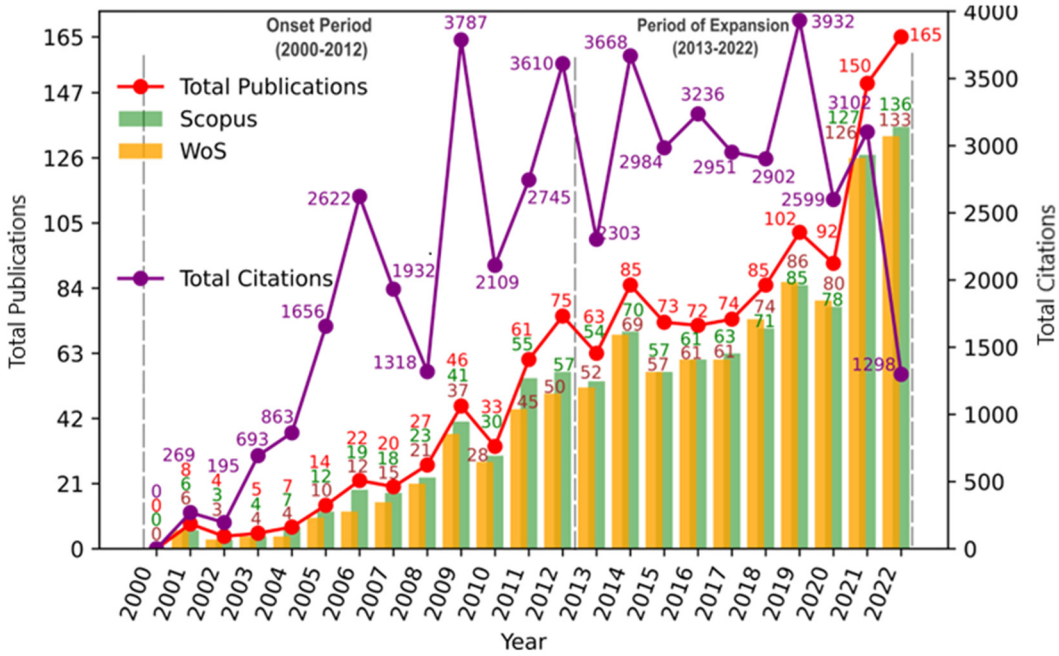

Fig. 1: Measurement of scientific production

porous materials has been assessed using Canonical Monte Carlo modeling. However, the accuracy of the mentioned simulations is directly related with the accurate description of the force fields that mimics the interatomic interactions. Three strategies are highlighted to improve H_2 gas phase storage capacity in MOFs and COFs, such as the incorporation of adsorption sites of transition metal into the organic bond through the Kubas interaction. Conversely, this phase emphasizes the significant importance of the H_2 oxidation reaction (HOR) and the hydrogen evolution reaction (HER) in advancing the hydrogen economy and facilitating the shift towards more sustainable energy sources. These reactions are essential for various reasons. Firstly, the HOR is used in fuel cells, which convert the chemical energy of H_2 into electricity efficiently and with minimal emissions, thus contributing to the reduction of the carbon footprint. Secondly, the HER enables the production of H_2 from water through electrolysis processes, facilitating its storage and transportation as a renewable energy source. Moreover, these reactions are vital for the advancement of clean energy technologies like fuel cells and electrolyzers, which are critical for the development of a H_2-based energy system. Research in these reactions also try to improve the efficiency of energy storage and conversion processes, which could lead to lower costs and greater adoption of H_2-based technologies. The most cited work in this bibliometric report is that of Strmcnik *et al.* (2013), with approximately 847 citations, thus highlighting its significant importance in the academic context. This study addresses the challenge associated with the low kinetics observed in the HOR in alkaline environments, and the limitation to the progress of systems of alkaline fuel cell. The data reveal that the performance of the HOR can be improved by more than five times relative to the cutting-edge platinum catalysts that were in use at that period. In this sense, the Iridium (Ir) and $Pt_{0.1}Ru_{0.9}$ (Platinum (10wt%) and Ruthenium (90wt%) alloy) materials stand out, which achieve balance between active sites necessary for the dissociative-adsorption of H_2, and the generation of surface species hydroxyl (OHad). The study suggests that the oxyphilic sites on the Ir electrodes and on the PtRu systems, allows the adsorption and formation of OHad species, thus enhancing the reaction with H_2 intermediates adsorbed on the surface sites.

Stage 3: High productivity stage (2016 - 2022)

The third period marked a significant rise in productivity and consolidation in the thematic domain. At this stage, the number of publications reached its peak, and the citation count was notably high, similar to the figures recorded in stage 2 (Fig. 1). In this way, it is evident that research at this stage has also a high impact in the development of recent studies related to H_2 adsorption capacity, storage and computational modeling. At this stage, Feng *et al.* (2018), research stands out, with around 514 citations, where nickel sulfide (Ni_3S_2) nanotubes decorated with copper (Cu) nanodots and supported on carbon fiber were developed with the purpose of obtaining a non-precious metal electrocatalyst and evaluating the efficiency in the HER in alkaline systems. The results highlighted the improvement in the HER activity of Ni_3S_2 nanotubes decorated with Cu nanodots, attributed to an optimized adsorption and atomic desorption of H_2, consolidating them as promising catalysts for the efficient production of H_2. Furthermore, the research offers an in-depth analysis of the essential mechanisms that enhance the efficiency of the HER. Concurrently, it lays important foundations for design applications and the advancement of efficient catalysts linked to renewable energy technologies. These findings represent a significant advancement in the development of sustainable energy technologies, offering a promising approach for H_2 generation. The characterization and electrochemical evaluation of Ni_3S_2 nanotubes decorated with Cu nanodots provides valuable information for researchers engaged in catalyst development, addressing not only HER, but also other processes related to renewable energy conversion. The literature review carried out by Ahmed and Jhung (2017), also has a high relevance, with a number of citations close to 360. This review offers a comprehensive examination of MOFs and their applications in adsorption and separation processes, emphasizing the significance of H_2 bonding interactions. The review highlights the advantages of MOFs over other adsorbents, emphasizing their broader range of functionalities, chemical activities, and greater adjustability. The review also emphasizes the importance of theoretical calculations for predicting H_2 bonding properties and understanding adsorbate-adsorbent chemistry and offers new insights into the design and applicability of MOFs for specific adsorption purposes. Methodologies such as DFT and single and double coupled cluster techniques are widely utilized to investigate H_2 bonding interactions, especially in the context of adsorption studies involving MOFs. Furthermore, the paper discusses the fundamental H_2 interactions related with adsorption onto MOFs, especially in the context of studies of adsorption of H_2 in gas/liquid phases. The study emphasizes the significance of H_2 bonds in the adsorption process of gaseous compounds that include H_2, along with molecules that contain oxygen (O_2) and nitrogen (N_2) atoms. The review emphasizes the potential usages of MOFs in adsorption and separation by the use of H_2 bonding mechanism, showing their promising applications in various scenarios.

H_2 storage technologies

Among the widely used technologies for H_2 storage are ccompressed hydrogen gas storage (CGA), liquid hydrogen (LH_2), and solid storage (using hydrides and nanomaterials). CGA is frequently used as a storage option for transportation by compressing the gas to high pressures, which significantly boosts its energy density (Liu *et al*., 2021). This CAG storage technique offers rapid H_2 loading and unloading, though it causes an energy loss of roughly 13-18 percent (%) of its heat value. It is essential that containers used for H_2 gas storage are not only affordable and lightweight but also provide effective protection against hydrogen leaks (Omran *et al.,* 2022). The storage of LH_2 involves cooling H_2 to temperatures below -252.8 °C in cryogenic tanks, which requires significant energy expenditure and may result in boil-off losses. Due to its enhanced volumetric energy density, this technique is more effective than the storage of H_2 in gaseous or cryogenic forms. LH_2 is stored in containers designed to maintain temperatures below -240 °C and has been successful in commercial applications, including fuel cell vehicles (Langmi *et al*., 2022; Kumar *et al*., 2024). The concept of solid H_2 storage pertains to the application of solid materials capable of adsorbing hydrogen, facilitating its storage and transport. This process occurs through chemisorption, where H_2 molecules in the gas phase are physically adsorbed onto the surface of a metal or alloy and then decompose into two H_2 atoms. These atoms penetrate the metal block and settle into interstitial locations in the metal sublattice, leading

to the creation of hydrides. During H_2 desorption, the atoms in interstitial positions diffuse from the block to the metal or alloy surface and then combine to form H_2 molecules (Liu *et al*., 2021). Metal hydrides like magnesium hydride and lithium borohydride have the capability to store H_2 by bonding it with metal atoms. In contrast, MOFs utilize physisorption to retain H_2 within their porous structures. Other materials, such as doped polymers, zeolites, clathrate hydrates, metal nitrides and imides, hydrogen-graphene materials (HGMs), and capillary arrays, utilize different mechanisms for storing H_2 (Chen *et al*., 2021). Compared to other carbon materials, including CNTs, graphene is notable for its higher binding energy during the physisorption of H_2. Through the functionalization of graphene, fundamental properties such as chemical reactivity, specific surface area, porosity, and interlayer spacing can be adjusted. These modifications enhance its capacity to adsorb H_2 and decrease the energy barrier of the process (Jain and Kandasubramanian, 2020). The use of solid H_2 storage provides various advantages over other techniques, including greater safety, more convenient transportation, higher storage densities, elimination of high-pressure and low-temperature requirements, and cost-effectiveness. Consequently, it has become a major focus for research efforts (Ruihan *et al*., 2024). The scalability of H_2 storage methods is influenced by various factors, including initial and operational costs. Gaseous storage, although widely used, requires significant investment in compression infrastructure and tanks, which can limit its implementation in emerging markets. In contrast, although liquid storage delivers superior volumetric efficiency, it encounters limitations stemming from its elevated production and maintenance costs (Barthélémy *et al*., 2017). In contrast, solid storage presents a more economical long-term option, making it an attractive candidate for investments in research and development. The scalability of solid storage is noteworthy, allowing it to be utilized across diverse settings, including residential and industrial applications. It avoids the harsh pressure and temperature conditions associated with alternative methods, thus serving as a versatile option in the quest for sustainable H_2 energy (Ruihan *et al*., 2024). Additionally, the availability of advanced technologies and the maturity of production processes are determinants of the scalability of these methods. Compression technology has been available for a longer time, allowing for quicker adoption, while solid storage, which involves the development of new materials and adsorption techniques, may require more time to optimize. Finally, the influence of political decisions and energy policies is essential, with government incentives for renewable energy development serving to expedite the implementation of particular methods. On the legal front, the lack of clear regulatory frameworks and specific safety regulations creates uncertainty for investments, while complex permit and licensing processes can delay the progress of projects. Regulations regarding emissions and sustainability may favor cleaner technologies, such as solid storage, while subsidy or tariff policies could influence the economic viability of gaseous and liquid methods, thereby affecting their scalability in the market.

Computational modelling methods in H_2 adsorption

The prevalent computational strategies and DFT methodologies concerning H_2 adsorption are illustrated in Table 3. The application of DFT in examining the adsorption of H_2 on a range of materials has been prevalent, with various methodologies presenting unique advantages tailored to the characteristics of the system under consideration. DFT- generalized gradient approximation (GGA) is one of the most used approaches, especially with the perdew-burke-ernzerhof (PBE) functional, due to its ability to accurately predict adsorption energies on metal surfaces such as palladium (Pd), Pt, and nickel (Ni), providing a good balance between accuracy and computational cost. Conversely, while the local density approximation (LDA) in DFT offers a more straightforward computational approach, it generally underestimates weak interactions, such as those found in H_2 adsorption. As a result, its applicability is largely confined to simpler systems or those where electronic interactions are more pronounced (Liu *et al*., 2024). For materials that are more complex, such as metal oxides characterized by strong electronic correlations, the use of DFT combined with Hubbard corrections (DFT+U) markedly improves the representation of electronic interactions in systems containing d-electrons. This is especially important for H_2 adsorption on transition metal oxides, where electronic correlation is a crucial factor. Additionally, DFT which include dispersion corrections as vdW, usually knowledge as (DFT-D). Hybrid functional, such

Table 3: DFT methodologies used for calculating H_2 adsorption

DFT Methods	Main Features	Applications in H_2 Adsorption	Contributions to Advances in H_2 Adsorption
DFT-LDA	This approximation depends on the local density of the electron	Applications in systems where the H_2 interaction is weak or on clean surfaces.	Although it is computationally simpler, it underestimates weak interactions, affecting the precision in H_2
DFT-GGA	Exchange-correction functional as PBE	Widely used to study adsorption energies and metal surfaces.	Accurately predicts the adsorption energy of H_2 on metal surfaces such as Pd, Ni. Allows optimization of adsorption geometries
DFT+U	Modification of DFT to include corrections in materials with strongly correlated electrons.	Adsorption on metal oxides or surfaces with transition elements.	Improves predictions in materials with d-electrons, such as transition metal oxides, where H_2 adsorptions can involve more complex electronic interactions.
DFT-D	Includes vdW corrections (dispersive interactions).	Applied on surfaces where weak interactions play a crucial role (e.g., MOFs, graphene).	Improves H_2 adsorption calculations on porous materials and carbon where dispersive forces are significant.
Hybrid DFT as B3LYP	Hybrid functional that combine a fraction Hartree-Fock exchange.	Useful for studying more complex adsorptions and systems with strong electronic interactions.	Improves accuracy in predicting adsorption energies in systems with significant quantum and electronic correlation effects
Meta-GGA	Functional that consider information from the gradient and the second derivative of the density.	Applications on surfaces where a more detailed description of the H_2-solid interaction is required.	It provides better predictions of H_2 adsorption on surfaces that involve non-trivial interactions between H_2 atoms and molecules.
DFT+vdW	Explicit incorporation of vdW interactions in the calculations.	Modeling of H_2 adsorption on materials with porosities, such as nanotubes and MOFs.	It substantially improves calculations for adsorptions where dispersion forces are important, particularly in materials with large surface areas.

as becke 3-parameter Lee-Yang-Parr (B3LYP), further enhance the accuracy in predicting adsorption energies by combining Hartree-Fock approximation with DFT. Despite their higher computational costs, these approaches are vital for characterizing systems in which electronic and quantum correlation effects are particularly pronounced (Santra *et al.*, 2022). On the other hand, Meta-GGA functional such as Tao-Perdew-Staroverov-Scuseria (TPSS) and strongly constrained and appropriately normed (SCAN) provide a more detailed description of the interaction between H_2 and surfaces, offering an improvement over traditional GGA functionalsin terms of accuracy. Finally, DFT+vdW methods, which explicitly integrate vdW interactions, have been essential for modeling H_2 adsorption in materials with large surface areas or porous structures, where these forces play a fundamental role in adsorption stability and capacity (Mahyuddin *et al.,* 2020).

Production by country

Currently, scientometric analysis of countries has established itself as a conventional tool to identify the most productive areas globally in relation to scientific areas. It is vital to comprehend the dynamics of scientific and academic output and to evaluate the quality and its effects in different nations. The current research outlines the production of scholarly work as indicated by the volume of articles, the quality determined through Scimago metrics, and the impact gauged by citation frequency in relation to a specific country. Worldwide collaborations are predominantly observed among developed countries. In this context, leading researchers from these nations are working together to develop new technologies aimed at mitigating pollution

Table 4: Most productive countries

Country	Production		Citation		Q1	Q2	Q3	Q4
China	435	24.96%	7981	21.38%	226	51	35	7
India	192	11.02%	3041	8.15%	105	22	13	3
United States	134	7.69%	5649	15.14%	85	6	5	0
Iran	90	5.16%	1447	3.88%	37	22	14	5
Japan	58	3.33%	1321	3.54%	38	9	3	0
Germany	56	3.21%	1367	3.66%	31	3	0	0
France	44	2.52%	1025	2.75%	29	4	1	0
Korea	41	2.35%	1196	3.2%	31	3	0	1
Australia	40	2.29%	1203	3.22%	30	2	0	0
Saudi Arabia	37	2.12%	260	0.7%	12	9	3	4

and reducing the impact of non-renewable energy sources, such as oil and fossil fuels, through the use of H_2. Likewise, a network for collaboration is created to comprehend the communities that emerge from the interactions among researchers. From 73 to 89 countries (Scopus and WoS, respectively) are involved in research and publication on the topic of H_2 adsorption and storage, using the DFT methodology in their respective studies. The initial ten articles are displayed in Table 4, arranged according to the number of publications. This order illustrates the involvement of the most prolific countries concerning the overall total of papers generated in this research. The first ten countries represent 64.65 % of scientific production, with China, India and the United States as the countries with the major number of contributions considered as relevant by the parameters employed. The explanation for this observation lies in one of the most frequently referenced from these countries, especially in China, that suggests a novel generation of materials designed to improve the reversible storage of hydrogen at ambient temperatures and moderate pressures (under 20 bars). In this context, it is reported that the system of graphene sheets with lithium (Li) pillars presents 6.5 wt% of storage capacity of H_2 under the operating conditions mentioned above, thus meeting the objective of the Department of Energy (DOE) in relation with storage materials for application in transportation (Deng *et al*., 2004). It is important to highlight that this work is authored by an individual of Chinese descent who has ties to the United States. However, the scientometric analysis identifies China as the country of origin of the study. Along these same lines, researchers from India carried out a review focused on the application of graphene, graphene oxide functionalized and their variations in applications of H_2 storage, supported by significant theoretical advances through DFT modeling and calculations, first principles calculations and Monte Carlo models, among other methods. Graphene in its pure form has deficiencies in H_2 storage, and the insertion of replacement of atoms into the structure of the material for dopants such as boron (B) and N_2, as well as decoration with transition metals, substantially improves its performance. Furthermore, graphene's capability to alter the curvature of its surface is identified as a significant factor that can facilitate the advancement of hydrogen storage systems with enhanced kinetics and reversible characteristics (Jain and Kandasubramanian, 2020). The work developed by Seenithurai *et al*. (2014), based on DFT calculations, revealed that double-vacancy graphene, effect of Li atoms decoration, calculations predict that this material serve as a plausible H_2 storage material. Likewise, it was highlighted that they achieved the maximum adsorption of four H_2 molecules in relation of one Li atom, this studied system generates a storage capacity of 3.89 wt%, and an energy of adsorption of 0.23 electron Volt per H_2 molecule (eV/H_2). The investigation carried out by Song *et al*. (2017), related with a bimetallic imidazolate zeolitic framework based on cobalt and phosphide (BCP-ZIF) with optimized composition was synthesized, stands out. This material acted as a bi-functional catalyst, facilitating the total decomposition of water by supporting both the HER and the oxygen evolution

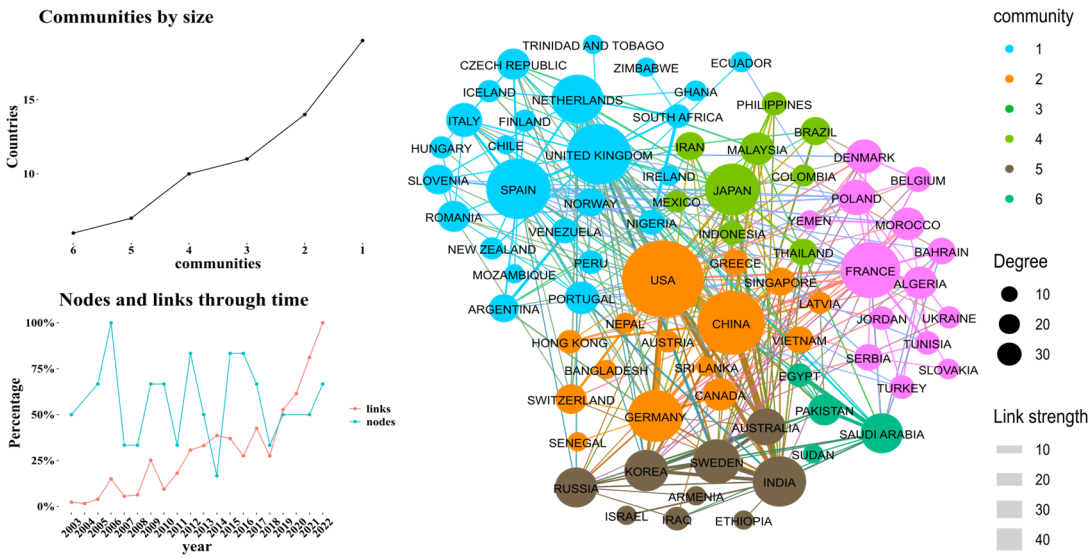

Fig. 2: Collaboration between countries

reaction (OER). Based on the results obtained, it was determined that $Cu_{0.3}Co_{2.7}P$/NC (copper (0.3) cobalt (2.7) phosphide supported on nitrogen-doped carbon) shows to be the most efficient BCP-ZIF bifunctional electrocatalyst for both HER and OER and demonstrates great potential for the electrolysis of water. The paper highlights the importance of H_2 production as a sustainable fuel produced using water electrolysis as the most practical solutions for energy conversion. This study's outcomes could greatly influence the progress of renewable energy development and the movement towards more sustainable energy solutions. On the other hand, Ferrin *et al.* (2012) developed a theoretical study using DFT-GGA using ultrasoft pseudopotentials, these calculations were done to understand the H_2 interaction with different facets of transition metals. The analyzed materials, excluding silver and gold, demonstrated that H_2 adsorption on the surface is exothermic when compared to H_2 in the gas phase. Conversely, at the subsurface level, the dissociation of H_2 is less stable than its adsorption on the surface. The comparison between open and compact facets shows that the diffusion of H_2 dissociated is related to the stability of the final state in each diffusion case. Some metals, as Pd, tantalum (Ta) and the case of vanadium (V), showed that the occupation of H_2 dissociated into the subsurface is an exothermic process with respect to H_2 in gas phase, thus favoring surface insertion from an energetic point of view. This tendency to favor subsurface sites is consistent with the industrial utilization of these metals, notably in applications involving H_2 membranes.

The six clusters of countries shown in Fig. 2 demonstrate that the size of each cluster reflects similar dimensions among most of the subgroups. The representation of nodes and nets along the time provides insight in the interaction between recent countries and the emerging relations that emerge along the time. Among the most relevant interactions are those of the United States, China, Spain and the United Kingdom (UK). The increase in research relationships in recent years is also highlighted, left-bottom graph.

Author production

When analyzing authors production presented in Table 5, it is evident that Ahuja is the most relevant author in Scopus and appears as the most influential author on the topic covered by this review. He is positioned in first place both in the number of publications and in citations received from other prominent authors in this field of knowledge. As an example of their work, the article published by Hussain *et al.* (2014), where polylithiated species (CLi_3: Trichlorolithium and CLi_4: Tetrachlorolithium)

Table 5: Production of articles by Scopus author

No.	Researcher	Total articles*	Scopus h-index	Affiliation
1	Ahuja R	20	91	Uppsala University, Sweden
2	Hussain T	15	44	The University of Queensland, Brisbane, Australia
3	Chakraborty B	15	34	Homi Bhabha National Institute, Mumbai, India
4	Juan A	13	26	IFISUR, UNS-CONICET, Argentina
5	Ruangpornvisuti V	11	21	University, Bangkok, Thailand
6	Liu P	11	14	Normal University, Chongqing, China
7	Chattaraj P.K	11	66	Indian Institute of Technology Bombay, Mumbai, India
8	Benyoussef A	11	42	Materials and Nanomaterials Center, MAScIR Foundation, Rabat Design Center, Rue Mohamed Al Jazouli Madinat Al Irfane, Rabat, Morocco
9	Zhang H	10	29	University, Chengdu, China
10	Petrushenko I.K	10	15	Technical University, Russian Federation

were employed for the functionalization of hydrogenated graphene (CH) as an efficient H_2 storage material. CH demonstrates significant promise as a hydrogen storage medium at the nanometric level due to its remarkable stability and its strong binding of H_2 atom with metals. The powerful interaction promotes a uniform spread of polylithiad dopants throughout the surface, which is beneficial for the functionalization of nanostructures. It was found that the functionalization of both sides of CH with CLi_3 and CLi_4 allows reaching a storage capacity that exceeds 13 wt% of H_2. In these cases, the adsorption energies range the 0.25 to 0.35 eV, these energies are suitable interactions for efficient H_2 storage. Later, Banerjee *et al*., 2016 presented a research on the potential of a functionalization with Li atoms of the materials known as a hydrogenated hexagonal boron nitride (BHNH), these materials is a system with shape of sheet, and it is expected to be applied in H_2 storage. The study employs a first-principles DFT technique to examine Li-substituted BHNH sheets, considering the key structural interactions, their energetic stability, and their current performance as H_2 storage, due to its capacity approximately (~) ~6wt%, a moderate binding energy with H_2 molecules (∼0.18- 0.3 eV) and favorable desorption kinetics. It has been reported that graphitic carbon nanosheets functionalized with light metals Li, sodium (Na), Ni, potassium (K), calcium (Ca), scandium (Sc), and titanium (Ti) are also promising materials for H_2 storage. A uniform distribution of light metals was observed on the nanosheets, resulting in a shift in their electronic properties from semiconductor to metallic. Furthermore, it has been observed that H_2 adsorption on the aforementioned nanosheets achieves a notable storage capacity of 6.5%. The energies of the adsorption interactions are within a favorable range for H_2 storage applications, as highlighted by Panigrahi *et al*. (2018). Carbonaceous materials such as graphitic carbon nitride (g-C_3N_4), materials already treated with N_2 presents uniform pores, are a promising option for storage of H_2. Also g-C_3N_4 has raised an attractive adsorptive material for H_2. The characteristics of this material can be attributed to its porous structure, which facilitates the entry of H_2 molecules. Additionally, the presence of double-bonded N_2 as a singular dissociated atom within the g-C_3N_4 framework, located at the pore edges, provides active adsorption sites for H_2. This interaction can occur either through chemical or physical means, or via functionalization with metallic dopants. Considering the interesting properties of g-C_3N_4, DFT with dispersion corrections including vdW interactions to explore the structural properties, electronic structure, mechanism of transfer of electron charge and H_2 adsorption on transition metal functionalized g-C_3N_4 sheets (Sc, Ti, Ni, V) have been presented. It was evidenced that the decoration of the g-C_3N_4 sheets with the metals and their dimers resulted in a high gravimetric density of H_2, with an

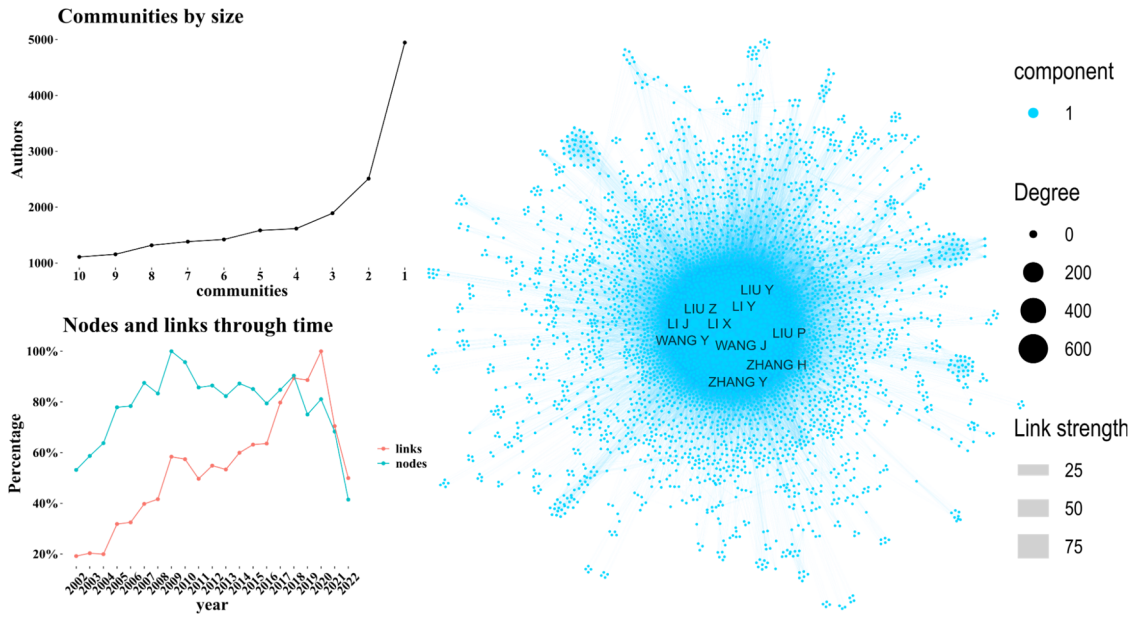

Fig. 3: Academic social network

optimal binding energy for practical applications. Furthermore, the thermal stability of these sheets was confirmed by molecular dynamics. Decoration with dimers turned out to be even more efficient for storage of H_2, with a binding energy per H_2 molecule thar ranges the 0.6 to 0.9 eV per molecule. Finally, the H_2 adsorption process on these sheets demonstrated a notable enhancement in the H_2 storage capacity as stated by Panigrahi *et al*. (2018).

The key authors pertinent to H_2 adsorption, storage, and computational modeling are depicted in Fig. 3, which showcases the most cited research communities. This analysis reveals the presence of ten identifiable communities focused on research and collaboration. The community referred to as "one" boasts the highest concentration of researchers and the most notable contributions, with a total of eight members included in the list. the community number one, present the most cited researchers such as Wang and Li, with a remarkable impact in the scientific community and higher connected networks even with new and with previous authors as Zhang and Chen that have had a greater impact belonging to community 2.

Production by journals

The publication of articles related to H_2 adsorption, storage and computational modeling, addressed in this review, reveals a set of journals that with a remarkable number of publications into the subject (Table 6 and Fig. 4). The International Journal of Hydrogen Energy is one of the most relevant journals. This journal is dedicated to exploring the application and research of technological innovations pertaining to hydrogen energy within the scientific field. The significance of original research lies in its comprehensive exploration of H_2 energy, effectively combining analytical methods with experimental techniques to address key factors. This includes H_2 production, H_2 storage, H_2 transmission, H_2 use and the environmental impact and the economic and worldwide aspects of H_2, including its carriers such as ammonia (NH_3), methane (CH_4) and alcohols, among others. It should be emphasized that, despite achieving the highest figures in terms of publication count and impact factor, this journal does not hold the top h-index among the publications that focus on the relevant topic. In this sense, reference can be made to the Journal of Physical Chemistry C, is in the highest site of the rank talking about h-index and the second site in the list, takin into account the number of publications of H_2 storage and adsorption. The mentioned journal is devoted to publishing

Table 6: Number of papers published in the main journals

Journal	WoS	Scopus	Impact Factor	h-Index	Quantile
International Journal of hydrogen Energy	250	262	1.32	248	Q1
Journal of Physical Chemistry C	61	60	1.03	323	Q1
Physical Chemistry Chemical Physics	44	40	0.82	272	Q1
Applied Surface Science	39	39	1.19	219	Q1
Computational and Theoretical Chemistry	18	18	0.38	96	Q3
Journal of Alloys and Compounds	17	17	1.08	200	Q1
Chemical Physics Letters	17	16	0.48	248	Q2
Journal of Molecular Modeling	16	15	0.36	76	Q3
Molecular Physics	13	13	0.38	114	Q3
RSC Advances	16	13	0.68	189	Q2
Global Journal of Environmental Science and Management	10	11	3.1	33	Q1

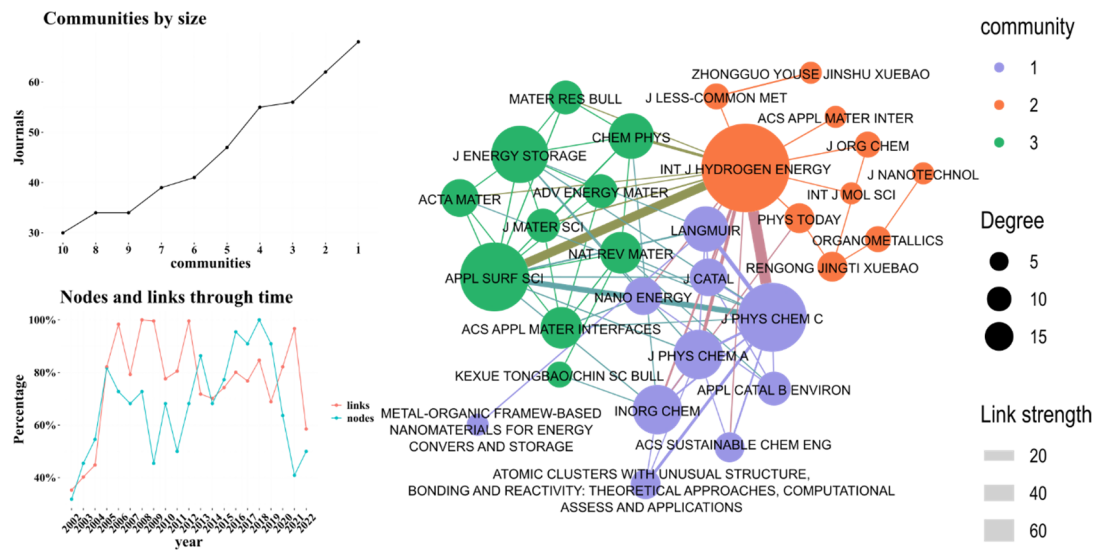

Fig. 4: Production by journals

experimental, theoretical and computational investigations focused on the physical-chemistry of nanoscale and low-dimensional bulk materials, as well as transformations at interfaces with chemical treatments. In addition, it addresses studies related to energy conversion and storage.

The Journal of Physical Chemistry Chemical Physics deserves special mention for its concentration on experimental and computational investigations in fields such as catalysis, surface science reaction mechanism, nanoscience, energy and surfaces/ interfaces among other. This journal prioritizes the synergy between experimental and theoretical investigations, showcasing those that complement each other and are informed approaches. It is important to highlight that the three previously mentioned journals, according to the bibliographic databases (Scopus and WoS), are classified in the first quartile and have the most outstanding metrics in the thematic area addressed in this review.

Production by keywords

Fig. 5 shows the most used keywords for the search of information on the topic under study. The most used keywords are "density functional theory", which appear in 581 documents. One of the most cited works where DFT calculations are used as key words was the work carried out by Kou *et al*. (2020). This work outlines a method to activate nickel oxide (NiO) via carbon doping, leading to the creation of poorly coordinated nickel sites that promote the adsorption of H_2. DFT studies shows that the insertion of doping atoms into carbon structures reduces the barrier of energy of the Heyrovsky mechanism from 1.17 eV to 0.81 eV. The mentioned results show that carbon possibly also acts as a reactive site for the water dissociation in the electrolysis process. At the other hand, the carbon doped with NiO catalyst showed a low overpotential of 27 millivolts (mV) at 10 milliampere per square centimeter (mA/cm²) of current density. In a similar vein, the Tafel mechanism demonstrates a slope of 36 millivolts per decade of current density (mV/dec), showcasing the highest efficiency among emerging NiO catalysts for H_2 production. The Pd, used in industry as a catalyst in hydrogenation reactions and exhaust gas cleaning (McCue and Anderson, 2015; Xu *et al*., 2022). It is unique among metals due to its high ability to split H_2 and its great solubility in this element in its total mass. The Pd behavior is known that at the presence of H_2 can modify parameters as the adsorption heat and the amount of H_2 that adheres to the surface (Johansson *et al*., 2010; Konda and Chen, 2016). A variety of computational investigations utilizing DFT have provided insights into the electronic properties of Pd surfaces and their key interactions with H_2. In general, density of states, electron densities, charge densities and local density of states are reported in the computational calculations (Camacho-Mendoza and Cruz-Borbolla, 2020; Huang and Chen, 2022; Xu *et al*., 2024), and the adsorption energy for several H_2 coverages and surfaces is studied (Kim *et al*., 2020; Rezaei and Najafi Chermahini, 2020; Singla *et al*., 2021; Zhou *et al*., 2020). The values of energy of adsorption at low coverage are in the ranges from 83 to 138 kilojoule per mole (kJ/mol) of H_2 (Amaya-Roncancio *et al*., 2022, 2018; Gómez *et al*., 2017). Likewise, the computational analyses concerning HER and their atomic-level ramifications as a cluster were thoroughly discussed by Xu *et al*. (2023). In the same line, green H_2 production perovskite-based materials, and their molecular implications are carefully observed in Guan *et al*. (2023).

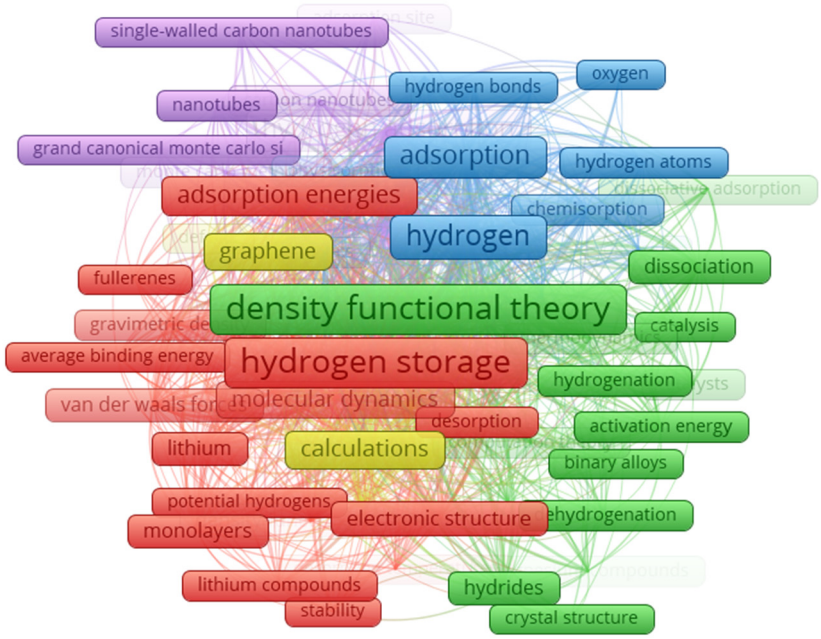

Fig. 5: Map of keyword occurrences

The second most used keywords are "hydrogen storage" which are present in 553 documents, among which the reported paper of Mpourmpakis *et al*. (2006), who report a multi-scale theoretical approach to research H_2 storage in SiCNTs nanotubes, stands out. Research utilizing ab-initio calculations and Monte Carlo modeling has revealed that silicon SiCNTs exhibit superior hydrogen storage capabilities relative to pure CNTs. The quantity of H_2 stored depends on the long range interaction between the atoms that conforms the tube and the H_2 molecules. The analysis of H_2 storage in the synthesized CNTs was conducted using a multiscale theoretical approach in conjunction with the calculations referenced earlier. The results indicate that the synthesized nanotubes could fail in the moment of H_2 accumulation because of the distance between layers, that from calculations and experimental observations shows to be small in comparison with the amount of H_2 molecules to be introduced. However, and spiral structure of about 7 ångström (Å) in conjunction with alkaline doping could improve the performance of this materials for H_2 storage application. In the last case, the material reaches 3 wt% at room temperature and environmental pressure (Mpourmpakis *et al*., 2007). Along the same lines, the H_2 reversible storage mediated by CO_2 has been corroborated by heterogeneous catalyst of Pd in conjunction with mesoporous graphitic (mpg) supported carbon nitride (Pd/mpg-C_3N_4). This catalyst demonstrated significant activity to produce H_2 from formic acid (FA), the reaction involved was free of additives and was driven in ambient conditions. The increase in catalytic efficiency is likely due to the quantity of nitrogenated functional groups found in mpg-C_3N_4. It is mentioned that the nitrogenated groups stabilize the Pd nanoparticles and generate basic sites for FA activation. Moreover, the inclusion of triethylamine allowed this catalyst material to show selectivity in the synthesis of FA. Here, the reaction sites of the support material could induce the interaction with CO_2 for the synthesis of FA (Lee *et al*., 2014). The term *'hydrogen'* is in the third position among the most used keywords in this review, which is reported in 338 articles. A highly referenced study (570 citations) is by Bluhm *et al*. (2006), which explores the improved dehydrogenation of amineboranes, particularly ammonium borane, in ionic liquids, presenting it as a viable approach for chemical H_2 storage. It indicates how ionic liquids, such as 1-butyl-3-methylimidazolium chloride (bmimCl), can improve the rate and extent of ammonium borane dehydrogenation. This effect could also be related to the formation of polarized ionic functional groups. The case of computational modeling for H_2 adsorption and dissociation, there are several methodologies implemented along the years. The accuracy of these calculations is generally related to their computational cost (Grajciar *et al*., 2018; Kroes, 2021). Within the realm of ab-initio calculations, the fundamental methodologies for achieving accurate calculations are typically outlined. Adsorption geometries for H_2 on pyrene and B-doped pyrene, by the use of Møller-Plesset theory and restricted open Hartree-Fock calculations were implemented as an accurate approximation in the early decade of 2000-2010, to characterize the H_2 adsorption on and graphene surfaces (Hübner *et al*., 2004; Wexler *et al*., 2010). In a similar vein, DFT calculations have been employed to investigate H_2 adsorption and the movement of hydrogen atoms on graphene, along with their diffusion across metal surfaces (Casolo *et al*., 2009; Huo *et al*., 2005). Hartree-Fock calculations calculations and their variants can take a long time for calculation, and a limited number of atoms can be represented in their models. Although molecular dynamics is not linked to ab initio calculations, it offers significant information and facilitates the modeling of numerous atoms and molecules. This methodology is effective for exploring the interactions between H_2 with various adsorbent surfaces (Yu *et al*., 2022). The molecular dynamics models usually require high memory capacity, and the dynamic information can generate noise. DFT is an approximation based on the solution of the Khon-Sham equations. Its variants can improve the level of accuracy of their models in comparison to Hartree-Fock models, but with less time calculation. DFT have been widely used over the last two decades for understanding the fundamental aspects of atomic interactions (Cohen *et al*., 2012; Mardirossian and Head-Gordon, 2017). A high level of accuracy can be attained when calculating H_2 adsorption in the contexts of chemisorption and physisorption interactions (Amaya-Roncancio *et al*., 2018; Silveri *et al*., 2019). H_2 adsorption properties on the surface and subsurface of transition metals and near-surface alloys (NSAs) using DFT calculations are discussed (Greeley and Mavrikakis, 2005). The formation of H_2

at the surface is generally characterized as exothermic in NSAs and pure metals, while at the subsurface level, it is typically endothermic, except in the case of pure Pd. NSAs showed a combination of catalytic mechanisms for hydrogeation reactions, with not binding H_2 energies that would allow to operate at low temperatures and low H_2 dissociation barriers, near to exothermic and non-activated process, would make them active for hydrogenation processes. A clear linear correlation was observed between the density of electronic states of the NSAs and the binding energy of H_2 on both the surface and subsurface. This indicates that the electronic structure plays a crucial role in determining the H_2 adsorption characteristics in these systems (Greeley and Mavrikakis, 2005). The words "*gas adsorption*" are in the fourth position of the most used keywords in this research topic (present in 311 articles). In this sense, in the work of Islam *et al*. (2011), the adsorption and diffusion of H_2 on the surface of anatase phase of titanium dioxide (TiO_2) (101) was analyzed using DFT calculations. Utilizing periodic DFT and DFT+U corrections, the interaction of H_2 across different surface positions has been examined. Results show that the adsorption of H_2 on the TiO_2 surface facilitates electron transfer to the Ti 3d states, thereby impacting the band structure. Transition state search methods were used to study H_2 diffusion, revealing the importance of electronic localization in the accurate description of these systems. The results apports valuable information on the hydrogen production using titanium dioxide (H_2-TiO_2) interaction, crucial for catalysis and energy storage applications. Another document that shows the use of these words is the one reported by Zhen *et al*. (2016), who presented a new efficient cocatalyst, NiMo@MIL-101 (Nickel and molybdenum confined into the metal-organic framework MIL-101), to improve the photocatalytic activity of the HER. The study focuses on the synthesis and in-depth characterization of the cocatalyst, showcasing its remarkable effectiveness in H_2 generation under visible light irradiation. This capability is attributed to the specific interaction of nickel-molybdenum (Ni−Mo) clusters with the active sites of the MOFs, which aids in the efficient transfer of electrons throughout the reaction process. The results also showed lower adsorption energy, higher apparent quantum efficiency, and higher stability compared to Ni@MIL-101 (Nickel confined into the metal-organic framework MIL-101) and Mo@MIL-101 (Molybdenum confined into the metal-organic framework MIL-101) catalysts. The NiMo@MIL-101 catalyst also exhibited a lower overpotential, a rise in transient photocatalytic current, and an extended fluorescence lifetime, emphasizing its importance in the context of visible photocatalytic H_2 production. The word "*adsorption*" occupies the fifth position of the most used terms in publications on the topic under study (used in 232 research works). A significant contribution to the literature on this topic is the article by Zhou *et al*. (2006). In their study, they investigated how doping with B and N_2 influences the adsorption of H_2 on a single-walled carbon nanotubes (SWNTs) using DFT calculations. It was observed that B-doping generates electron deficiency in the SWNTs structure, while the doping with the N_2 as atom forms a structure rich in electron density at the surface. Adsorption of H_2 on B or N_2 atoms modifies the electron density distribution on the tube wall, resulting in variations in the band structure and the energies associated with H_2 atomic adsorption. B doping significantly increased the H_2 adsorption capacity, while N_2 doping has a more moderate effect. In contrast, the interaction between H_2 molecules and the surfaces of transition metals holds considerable importance in heterogeneous catalysis and the synthesis of metal hydrides (Jiang and Carter, 2003; Schauermann and Freund, 2015). Transition metal surfaces can handle with a high number of hydrogenation reactions. The chemisorption of H_2 on iron (Fe) is a milestone in these studies, not only as a reagent in the Fe catalyzed synthesis of ammonia He *et al*. (2016), the Fischer-Tropsch reaction (Zhao *et al*., 2018), among others. In this sense, the H insertion into the bulk of the metal systems also weaken steels (Chohan *et al*., 2016; Ohaeri *et al*., 2018), this weaken can cause fracture and failure of the steel. Research into the adsorption of H_2 on iron surfaces has been conducted for several years (Bakulin *et al*., 2014; Boateng *et al*., 2017; Shen *et al*., 2016; Wang *et al*., 2014), demonstrating that molecular H_2 adsorbs dissociatively on the surfaces and is strongly exothermic process.

CHALLENGES AND OPPORTUNITIES

Based on the literature, it is observed that the primary challenge in H_2 storage is the low values of energy density of H_2 when it is stored at atmospheric

pressure and room temperature, which necessitates solutions for storing useful quantities in reasonable volumes. One of the key challenges in H_2 storage is sourcing materials that are safe, effective, and cost-efficient. Furthermore, computational research can offer insights that improve our comprehension of this domain. It is noteworthy that there has been a scarcity of collaboration between experimental and theoretical approaches, highlighting a vast potential for exploration and synergy in developing theoretical-experimental studies. Additionally, storing H_2 at high pressure poses significant safety risks, including leaks and explosions. Finally, the creation of infrastructure for the production, storage, and distribution of H_2 is costly and requires substantial investments. To address these challenges, the use of metal hydrides, which allow for higher storage densities through reversible chemical reactions, is one approach. Storing H_2 in the form of cryogenic liquid at extremely low temperatures is another option, though it involves high energy costs to maintain the temperature. The evolution of carbon-based materials, like CNTs and graphene, presents enhanced storage capabilities owing to their porous design. Research into chemical compounds, such as borohydrides and ammonia, which can release H_2 through catalytic processes, is also promising. CNTs and electrocatalysts have revolutionized H_2 storage by offering more efficient and safer solutions to overcome traditional challenges in this area. Owing to their unique cylindrical configuration and significant surface-to-volume ratio, CNTs possess an outstanding capability for hydrogen adsorption, facilitating the storage of more gas than other materials can achieve. Their lightness makes them ideal for applications where weight is a critical factor, such as in transportation, and their mechanical and thermal stability allows them to withstand high-pressure conditions while maintaining optimal performance. Furthermore, modifications can be made via doping or chemical functionalization, which enhances their ability to adsorb and allows for hydrogen storage at lower pressures, resulting in a safer and more efficient process. Electrocatalysts have played a fundamental role in improving the efficiency of H_2 production and storage processes, particularly in water electrolysis, where they facilitate the reactions that separate water molecules to produce H_2 and O_2. Metal-based electrocatalysts such as Pt, along with more economical alternatives like Ni- or Co-based electrocatalysts, have significantly improved the speed of electrochemical reactions and the energy efficiency of the process. This development has allowed for the production of H_2 to be cleaner and quicker, a vital factor for its storage and future utilization in applications including. The environmental effects of producing and using materials like CNTs and graphene for hydrogen storage necessitate a comprehensive life cycle analysis (LCA). The synthesis of these advanced materials often involves energy-intensive processes, such as chemical vapor deposition, which can lead to significant carbon emissions and hazardous byproducts. Additionally, the extraction of raw materials for CNTs and graphene production may result in habitat destruction and water pollution. These materials exhibit remarkable qualities for H_2 storage; however, their disposal or recycling raises ecological concerns, since improper disposal can contribute to microplastic pollution. Therefore, assessing the environmental impacts at each stage-from production to disposal-is crucial for identifying strategies to mitigate negative effects and enhance the sustainability of hydrogen storage technologies. The deployment of H_2 storage technology holds considerable political and economic significance, which may lead to a reconfiguration of the energy landscape and shift global geopolitical relations. Politically, it could lead to energy decentralization and reduced reliance on fossil fuel imports, disrupting current geopolitical dynamics dominated by natural resource-rich countries. H_2 can be locally produced from renewable sources, redistributing energy power and enabling more nations to achieve energy independence. The change could incite tensions in regions reliant on oil and gas production due to falling revenues, while also giving rise to new partnerships and disputes as countries with renewable energy assets and sophisticated hydrogen technologies become influential players. National and international energy and environmental policies would need to foster H_2 adoption by supporting decarbonization efforts, incentivizing investment in H_2 infrastructure, and balancing subsidies between renewable energy technologies. From an economic perspective, it is anticipated that production costs will decline due to the falling prices of renewable energy and advancements in electrolyzer technologies. Large-scale infrastructure for H_2 storage and transport requires significant

investment but could benefit from economies of scale in the long run. H_2 may demonstrate economic feasibility in industries facing significant challenges in decarbonization, such as chemicals, steel, cement, and heavy transport. Nevertheless, its effectiveness in the transportation sector is uncertain, largely because of the competitive edge of electric batteries. Government subsidies, private sector financing, and the establishment of carbon markets will play a crucial role in enhancing the economic viability of clean H_2.

CONCLUSION

A review of the development of research focused on H2 adsorption and storage, informed by DFT calculations, shows a notable growth in scientific contributions throughout the years. The initial stage (2000-2008) laid the foundation with fundamental works on ionic liquids and H_2 storage, while the intermediate stage (2009-2015) witnessed a significant increase in publications, with a four-fold increase in citations compared to the first stage. The current stage (2016-2023) shows maximum productivity, with cutting-edge studies on nanotubes and electrocatalysts driving advancements in efficient H_2 evolution. Collaborative networks on a global scale have been instrumental in transforming the research landscape, highlighted by a significant growth in partnerships among researchers from different nations. The analysis identified influential authors and top journals, with key researchers garnering significant citations and high impact publications. The synergy of collaborative research has resulted in a more unified research community, enabling the flow of knowledge and hastening progress in H_2 storage technology advancements. The BA provides quantitative insights into the trends and collaborative dynamics that have defined the evolution of DFT calculations in H_2 adsorption and storage research. The impressive tally of more than 9,548 citations in subsequent research highlights the establishment and recognition of this thematic area in the field of academia. Identification of influential authors and top journals underscores the impact of key contributors in advancing the field and disseminating critical research findings. An increasing focus has been identified in the development of advanced porous materials as MOFs and zeolites, which demonstrate significant potential for enhancing H_2 adsorption capacity and long-term stability. Recent studies have shown a trend towards optimizing these materials at the molecular level to maximize H_2 retention efficiency. Sustainable H_2 production, particularly through methods like electrolysis powered by renewable sources, is emerging as an area of significant interest. Findings suggest that there is a significant emphasis on innovating catalysts and integrating systems, with the primary goals of boosting energy efficiency and minimizing operational costs. In the future, integrating diverse research approaches and promoting interdisciplinary collaborations will be essential to drive advancements in H_2 storage technologies. By harnessing new technologies and focusing on the distribution of knowledge, the sector can confront complex issues and drive the development of effective and readily available H_2 storage solutions. To fully harness H_2 capabilities as a clean energy carrier and satisfy the rising energy needs of the future, sustained collaboration and innovation are crucial.

AUTHOR CONTRIBUTIONS

D.A. Torres-Ceron, the corresponding author, contributed to the design and conceptualization of the research, as well as to the revision of the manuscript. S. Amaya-Roncacio, participated in the supervision and manuscript preparation. F. Fuentes-Gandara, analyzed the results and contributed to writing the manuscript. E. Restrepo-Parra assisted in the conceptualization and revision of the manuscript. L. Bohorquez-Santiago, designed the manuscript's tables and figures and contributed to its revision. J. Velasquez-Tamayo, participated in writing - original draft

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CONFLICT OF INTEREST

The authors declare that there are no conflict of

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ABBREVIATIONS

°C	Degree Celsius
%	Percentage
~	Approximately
$[N_3H_8C]C+BH_4$	Methylguanidinium borohydride
Å	Angstrom
B	Boron
B3LYP	Becke, 3-parameter, Lee-Yang-Parr
BA	Bibliometric analysis
BCP-ZIF	Bimetallic imidazolate zeolitic framework based on cobalt and phosphide
BHNH	Hydrogenated hexagonal boron nitride
BminCl	1-butyl-3-methylimidazolium chloride
Ca	Calcium
CGA	Compressed hydrogen gas storage
CH	Hydrogenated graphene
CH_4	Methane
CLi_3	Trichlorolithium
CLi_4	Tetrachlorolithium
CNTs	Carbon nanotubes
CO_2	Carbon dioxide
COFs	Covalent organic frameworks
Cu	Copper
$Cu_{0.3}Co_{2.7}P/NC$	Copper (0.3) cobalt (2.7) phosphide supported on nitrogen-doped carbon
DFT	Density functional theory
DFT-D	Density functional theory with dispersion correction
DFT+U	Density functional theory with Hubbard parameter U
DOE	Department of Energy
EDA	Exploratory Data Analysis
Eq.	Equation
eV	Electronvolt
eV/H_2	Electronvolt by Hydrogen
FA	Formic acid
Fe	Iron
Fig.	Figure
GGA	Generalized Gradient Approximation
$g\text{-}C_3N_4$	Graphitic carbon nitride
H_2	Hydrogen
H_2TiO_2	Hydrogen production using titanium dioxide

HER	Hydrogen evolution reaction
HGMs	Hydrogen-graphene materials
HOR	Hydrogen oxidation reaction
Ir	Iridium
K	Potassium
kJ	Kilojoule
kJ/mole	Kilojoule per mol
LCA	Lifecycle analysis
LDA	Local Density Approximation
Li	Lithium
LH_2	Liquid hydrogen
MIL	Matériaux de l'Institut Lavoisier
Mo@MIL-101	Molybdenum confined into the metal-organic framework MIL-101
MOFs	Metal-organic frameworks
mA	Miliamperes
mA/cm²	Milliampere per square centimeter
mpg	Mesoporous graphitic
mV	Milivolts
mV/dec	Millivolts per decad of current density
N_2	Nitrogen
Na	Sodium
NH_3	Ammonia
NO_2	Nitrogen dioxide
Ni	Nickel
Ni–Mo	Nickel-molybdenum
Ni@MIL-101	Nickel confined into the metal-organic framework MIL-101
NiMo@MIL-101	Nickel and molybdenum confined into the metal-organic framework MIL-101
NiO	Nickel oxide
Ni_3S_2	Nickel sulfide
NSAs	Near-surface alloys
O_2	Oxygen
OER	Oxygen evolution reaction
OHad	Adsorption of hydroxyl species
PBE	Perdew-burke-ernzerhof
Pd	Palladium
Pd/mpg-C_3N_4	Palladium supported on mesoporous nitrogen-doped graphite carbon nitride
PRISMA	Preferred reporting items for systematic reviews and meta-analyses
Pt	Platinum
$Pt_{0.1}Ru_{0.9}$	Platinum (10%) and Ruthenium (90%) alloy
Ru	Ruthenium
Sc	Scandium
SiCNTs	Silicon-carbon nanotubes
SCAN	Strongly Constrained and Appropriately Normed
SO_2	Sulfur dioxide
SWNTs	single-walled carbon nanotubes
Ta	Tantalum
Ti	Titanium
TPSS	Tao-perdew-staroverov-scuseria
TiO_2	Titanium dioxide
UK	United Kingdom
V	Vanadium
vdW	van der Waals
WoS	Web of Science
Wt%	Weight percent

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