

## Exploring Technological Solutions for Onboard Hydrogen Storage Systems Through a Heterogeneous Knowledge Network: From Current State to Future Research Opportunities

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With the imminent threat of the energy crises, innovation in energy technologies is happening world-wide. The aim is to reduce our reliance on fossil fuels. Electric vehicles with fuel-cells that use hydrogen as an energy carrier are touted to be one of the most important potential replacements of the gasoline vehicle in both future transportation scenarios and emerging smart energy grids. However, hydrogen storage is a major technical barrier that lies between where we are now and the mass application of hydrogen energy. Further exploration of onboard hydrogen storage systems (OHSS) is urgently needed and, in this regard, a comprehensive technology opportunity analysis will help. Hence, with this research, we drew on scientific papers and patents related to OHSS and developed a novel methodology for investigating the past, present, and future development trends in OHSS. Specifically, we constructed a heterogeneous knowledge network using a unique multi-component structure with three core components: hydrogen carriers, hydrogen storage materials, and fuel cells. From this network, we extracted both the developed and underdeveloped technological solutions in the field and applied a well-designed evaluation system and prediction model to score the future development potential of these technological solutions. What emerged was the most promising directions of research in the short, medium, and long term. The results show that our methodology can effectively identify technology opportunities in OHSS, along with providing valuable decision support to researchers and enterprise managers associated with the development and application of OHSS.

Keywords: technology opportunities analysis, heterogeneous knowledge network, principal component analysis, network analysis, onboard hydrogen storage system

## **1 INTRODUCTION**

The imminent energy crisis and growing energy consumption is not only causing an unprecedented demand for reducing our reliance on fossil fuels, it is also prompting us to urgently explore new and sustainable energy carriers. Future energy carriers have to be efficient, clean, economical, and safe, and should allow for high volumetric and gravimetric storage densities (Abe et al., 2019; Tarhan and Çil, 2021). Hydrogen appears to be a very promising energy storage medium that may be a substitute

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for oil and other fossil fuels, and hydrogen fuel cells for vehicles is just one of its remarkable applications. Although electric vehicles are already considered a green solution in transportation scenario, vehicles equipped with a hydrogen fuel cell still outperform electric vehicle in several respects (Shi et al., 2019). First, most electrical power is generated by fossil fuels, while hydrogen is a zero emissions energy source. This means it can increase the environmental performance of power systems (Jannati and Nazarpour, 2018). Second, electric vehicles suffer from peak-time problems with the power grid, whereas hydrogen fuel cells have no such issues. However, there are two main barriers that lie between where we are now and the mass application of hydrogen energy. These are the ability to safely store hydrogen in sufficient quantities and devising the proper storage conditions for the energy produced.

Over the last 2 decades, research activities and innovation in the field of hydrogen storage has been driven by attempts to establish onboard hydrogen storage systems (OHSS) for cars powered by hydrogen fuel cells (Mori and Hirose, 2009; Weidenthaler and Felderhoff, 2011; Hwang and Varma, 2014). With the help of these researchers, hydrogen fuel cell vehicles have been put into small scale production (Nechaev et al., 2017). Although the market for mobile hydrogen energy storage continues to grow, further R&D efforts are still needed to achieve the desired energy and cost efficiency goals (Cumalioglu et al., 2008). Additionally, other aspects of OHSS, such as storage capacity, refilling times, and lifecycles, also need to be improved (Li M et al., 2019; Hassan et al., 2021). To actively respond to these changing technological requirements, we must understand the evolution and current state of technological development, explore new technological opportunities and research directions. Only this way will we further advance the globe's transition towards low-carbon energy and sustainable development (Aaldering et al., 2019).

Previous research sheds light on knowledge recombination as the theoretical foundation for the analysis of technological evolution and opportunities. It is widely known that innovation often originates from combining existing scientific and technological knowledge-commonly called knowledge recombination (Edquist, 1997; Xiao et al., 2021). By recombining existing knowledge elements in new ways, or finding new relationships between already-combined elements, new knowledge can be generated. In fact, knowledge recombination is often considered to be a "shortcut" to higher-level technologies that comes at a low switching cost (Frenken et al., 2012). As Antonelli et al. (2010) points out, the countries that achieve higher growth rates in productivity are usually those that have a superior ability to recombine technologies so as to generate new technological knowledge. Several scholars highlight that the existing knowledge surrounding a technology greatly affects where efforts toward innovation should be allocated, as well as which technologies are likely to be implemented in future practice (Wu and Shanley, 2009; Roper and Hewitt-Dundas, 2015). In this regard, several hydrogen storage technology areas are reviewed and analyzed based on the perspective of knowledge recombination. In recent years, some review researches of hydrogen storage technology

have been published, covering storage options (Elberry et al., 2021), materials and process design (Chanchetti et al., 2016; Turani-I-Belloto et al., 2021), energy carriers (Aziz, 2021) and fuel cells (Eriksson and Gray, 2017; Gong and Verstraete, 2017). Most studies have future-oriented feature, and have proved helpful to investigate development trends of hydrogen storage technology. Thus, understanding the knowledge existing in the field of OHSS is critically important when exploring future technological opportunities.

Technological knowledge can mainly be found in the science and technology (S&T) literature, i.e., scientific papers and patents (Li X et al., 2019). Using S&T information as data sources to obtain research opportunities seems a good way, especially in the energy storage field. Investigation shows that over 35% of technology opportunity analysis articles in energy storage technology are based on extant knowledge stock. Fundamental research in science is recorded by scientific papers, which act like seeds for the development of new technologies (Shibata et al., 2010). In previous studies, scientific data has been used as a data resource for recognizing research patterns (Ma et al., 2015), mining technical intelligence (Zhang et al., 2014), and monitoring technology development trends (Bakhtin et al., 2017). Patents, in addition to providing protection for inventions, are regarded as an up-to-date and reliable source of information reflecting technological advances and inventive activities (Kim and Lee, 2015). Surveys have shown that, patents contain up to 80% of the latest global technical information (Asche, 2017). For these reasons, patent data have been widely used to forecast technological innovation pathways (Zhou et al., 2018), formulate technology strategies (Yu and Zhang, 2019), analyze the interdisciplinarity of technology fusion (Ko et al., 2014), and visualize knowledge ecosystems (Schillaci et al., 2021).

Many empirical studies have indicated that the interdependence and interactions between science and technology have been increasing (Wang et al., 2015). Vast quantities of the latest technical information have been recorded and shared in scientific papers, which indicates that technological development is increasingly relying on science (Brandl, 1998). In fact, the progress of science is essentially exogenous, and technological advances are the result of R&D (Liu et al., 2018). This means technological application usually fall slightly behind scientific breakthroughs. Consequently, analyzing the gaps between scientific research and patents is an effective way of understanding the trends in technology innovation and can offer significant support when exploring technology opportunities (Yoon and Magee, 2018).

With the help of scientific and patent data, different wellestablished methods have been developed to measure S&T knowledge, such as a systematic literature review, content analysis, meta-analysis, bibliometric analysis, patentometric analysis, among others. These methods not only describe the S&T knowledge of a certain technology field in its current state, but also its origins and recombination dynamics. This helps to reveal the evolutionary trends in technology innovation (Avila-Robinson and Miyazaki, 2013; Gerdsri et al., 2013; Rodríguez-Salvador et al., 2017). However, most of these methods have not been very good at capturing the latent knowledge structures in S&T information. In order to explore the technological solutions for OHSS and to provide a deeper insight into current status and research opportunities in this field, different analyses should be performed. In semantic frameworks, technological knowledge can be defined as a collection of knowledge elements that represents the core knowledge of the corresponding technology field. In OHSS, the situation is more complex, as innovation is mainly reflected in the emergence of a new technological solution, which consists of a complete set of technological components. Each technological component is formed by a set of well-organized S&T knowledge. So, if the latent knowledge structures in the field are not revealed, the method is not likely to support further analysis well. Additionally, previous studies are more reliant on pre-defined technological topics when characterizing knowledge structures, which may result in the extreme risk of omitting important emerging knowledge with development potential.

In this study, using scientific papers and patents as a data source, we propose a novel methodology based on a heterogeneous knowledge network. The methodology reviews research progress of key and emerging technologies for OHSS from the period of 2008-2019, and provides an inclusive view of the technological solutions and innovations in OHSS. It also helps to predict the future development potential of technological entities and solutions. The analytical process of the methodology is as follows. First, principal components analysis (PCA) is applied to extract the principal technological components of OHSS from a list of unrelated technological knowledge elements. Then, based on the extracted technological components, a heterogeneous knowledge network representing OHSS is constructed. Through network analysis, we can identify the knowledge points that represent key and emerging technologies, and track their evolutionary dynamics. Then, a well-designed evaluation system measures and predicts underdeveloped and possible future technological solutions. Finally, short-term, medium-term and long-term technology opportunities of OHSS are obtained from the results. Overall, the picture developed provides insights for both researchers and enterprise managers in the field of OHSS. We expect that the insights revealed should prompt technology-oriented steps towards a low-carbon economy. Additionally, we expected that the proposed methodology will be helpful in exploring latent innovation opportunities and the development potential of not only OHSS, but also other technological fields.

The rest of this study is organized as follows. Section 2 describes the data and the proposed methodology. Section 3 outlines the network construction process and the process of identifying the technological solutions. Section 4 evaluates the development potential of those solutions. Section 5 provides the conclusion and outlook for future research.

## 2 DATA AND METHODOLOGY

The overall framework of our proposed methodology is illustrated in **Figure 1**. It contains five streamlined modules:

entity extraction, heterogeneous network construction, network analysis, the identification of technological solutions, and the evaluation and prediction of technological solutions.

## 2.1 Extracting the Entities

This module primarily extracts technological entities from scientific and patent data for subsequent analysis. Herein, a technological entity refers to any singular, identifiable and separate technique, method, material, tool or process used in the storage of hydrogen. The main steps of the entity extraction process are as follows.

Step (1) involves formulating a retrieval strategy to collect data related to OHSS. In Step (2), a natural language processing algorithm statistically analyzes the frequency of words and phrases (both referred to as words hereafter). The 500 most frequently used words are then selected and irrelevant words are manually eliminated. This refined set of words are now considered as keywords. In Step (3), keywords that ostensibly have the same meaning are merged to leave a list of unique technological entities. The entities in the unstructured text of the collected scientific papers and patents are then converted into frequency vectors, which can be used for document screening and further analysis. Finally, in Step (4), the entity vectors are analyzed and any documents that contain two or more entities are screened into the sample. The final result is a scientific dataset and a patent dataset of OHSS entity vectors.

## 2.2 Constructing the Heterogeneous Knowledge Network

In technology mining research, keyword co-occurrence networks are generally used to provide a topology of the potential relationships between technologies. However, most of these do not clearly indicate what kind of relationships they are, nor do they identify the knowledge structures in the given field. In this paper, we introduce a heterogeneous knowledge network to address this limitation that reveals insights into the knowledge structures of OHSS.

Heterogeneous knowledge networks can express detailed structured information with a focus on the interaction of core technologies by generating technological components for the selected technology field. In this network, the nodes are entities, and the technological components are clusters of technological entities of the same type (see Figure 2). Technological components represent the main types, or classes, of technological entities in the OHSS knowledge system. For example, technological entities such as hydrogen, ethanol and methanol belong to the component of energy carriers. Technological entities such as inorganic salts, metal hydrides and carbon nanotubes fall into the component of storage materials. Solid oxide fuel cells, alkaline fuel cells and direct fuel cells belong to the component of fuel cells. PCA is then applied to extract the essential components of OHSS. Through discussions with domain experts, we can identify the core technological components that constitute the knowledge structure of OHSS. The extracted technological components reflect mainstream hydrogen storage technologies described in the S&T text.





Additionally, the edges in the network represent connections between the different technological components; connections within the components are not included in this study. Compared to traditional network methods where any two nodes can connect to each other, here, the connections between nodes within the same component have been removed. This is because the most meaningful associations to us occur between the different components. An example of how heterogeneous knowledge networks using the multi-component structure might be effective is useful here. Below is an abstract of an article. Keywords are shown in bold, the codes in brackets represent their technological components.

The paper reviews the state of the art of hydrogen storage systems based on **magnesium hydride** (**M**), emphasizing the role of thermal management, whose effectiveness depends on the effective thermal conductivity of the hydride, but also depends on other limiting factors such as wall contact resistance and convective exchanges with the heat transfer fluid. For daily cycles, the use of phase change material to store the heat of reaction appears to be the most effective solution. The integration with fuel cells (**proton exchange membrane fuel cell (F)** and **solid oxide fuel cell (F)**) highlights the dynamic behavior of these systems, which is related to the thermodynamic properties of **MgH2** (**M**). This allows for "selfadaptive" systems that do not require control of the hydrogen flow rate at the inlet of the fuel cell.

There are a total of three distinct keywords in this text. Among them, proton exchange membrane fuel cell and solid oxide fuel cell represent fuel cells, and magnesium hydride (MgH2) represents hydrogen storage materials. In a traditional keyword co-occurrence network, connections would be generated between all of these nodes. However, a discussion on the relationship between proton exchange membrane fuel cells and solid oxide fuel cells seems unnecessary. By identifying the core technological components, we found that the research on the co-occurrence relationships between components have more significance than the co-occurrence within components. Capturing such associations between different components more accurately reveals the knowledge structures within OHSS. This allows us to more easily explore the interactions between key technologies and also to predict potential links. Therefore, using a heterogeneous knowledge network to present the knowledge structures of a selected technological field obviously reduces network redundancy since all edges in the network can be explained. An illustration of the network is provided in Figure 2.

These components were then represented as nodes (entities) in a weighted heterogeneous network, where the edges reflect the cooccurrence frequencies of pairwise entities at the document-level. An adjacency matrix was used to calculate edge weights, formulated as





$$A_{V_m^i V_n^j} = \begin{cases} DF(V_m^i, V_n^j) (if V_m^i and V_n^j co - occur in a document) \\ 0 \end{cases}$$

in which  $V_m^i$  is the *i* th node (entity) in the *m* th component,  $V_n^j$  is the *j* th node (entity) in the *n* th component, and  $DF(V_m^i, V_n^j)$  is the document co-occurrence frequency between  $V_m^i$  and  $V_n^j$ .

This network can also be represented as a graph

$$G = \left( V_K, E_{K(K+1)/2} \right)$$

where  $V_K$  is the node set of K technological components and  $E_{K(K+1)/2}$  is the set of K(K+1)/2 edges connecting the nodes between different technological components.

### 2.3 Analyzing the Dynamics of the Network

To analyze the evolution of the network, we divided the sample into three different time intervals (2008–2011, 2012–2015, and 2016–2019). This allowed us to track how the network developed over time (see **Figure 3**). Once we determined the number of core technological components in each interval, we were able to



TABLE 1 | Indexing system to evaluate the utility of entities.

Туре	Code	Evaluating index	Explanation
Technology importance index (I)	11	Average time for patent application	Sum(current_year-application_year)/N
	12	Keyword frequency in papers	The keyword frequency of each entity (papers)
	13	Keyword frequency in patents	The keyword frequency of each entity (patents)
	14	Total cited frequency	Sum (citation frequency of paper including the entity)
Technology potential index (P)	P1	Recent 3-years keyword frequency in papers	The keyword frequency of each entity in recent 3 years (papers)
	P2	Recent 3-years keyword frequency in patents	The keyword frequency of each entity in recent 3 years (patents

explore the overall changes in composition and concentration of the network entities. In this manner, the entities constituting each technological component highlight the degree of development in field. We tracked the dynamic of the heterogeneous knowledge network, and measured the core technological entities, entity pairs and emerging technological entities. To analyze the tendencies for key technologies to change, we used centrality as an indicator.

Centrality is a basic concept in network analysis. Different centrality indicators generally measure the importance or prominence of an element within a network in distinct ways. By identifying a central node, we can determine the key technologies of a field. Centrality includes three indicators, degree centrality ( $C^d$ ), betweenness centrality ( $C^b$ ), and closeness centrality ( $C^c$ ), which respectively reflect the node's capacity to aggregate, transfer, and disseminate information across a network. In our analysis, all three indicators proved to be effective in revealing the key technological entities in OHSS. Formal definitions for these indicators follow.

Degree centrality ( $C^d$ ): This indicator measures a node's direct influence on other nodes within a network by calculating the proportion of its degree (Borgatti, 2005). A technological entity with a high degree centrality indicates that it has strong direct connections or interactions with other entities, indicating that it is a key technology in the given field. The formula for calculating degree centrality is given by

$$C_i^d = \frac{k_i}{N-1}$$

where  $k_i$  is the degree of node *i* and *N* is the number of nodes.

Betweenness centrality ( $C^b$ ): This indicator measures the ability of a node to connect any other two nodes (Freeman, 1977). In a knowledge network, entities with high betweenness centrality are critical to controlling knowledge flows; hence, they are critical information transmitters in a network. Betweenness centrality is calculated by the fraction of shortest paths between



pairs of nodes in a network that go through the target node, which is given by

$$C_{i}^{b} = \frac{2}{(N-1)(N-2)} \sum_{p \neq i \neq q} \frac{n_{pq}^{i}}{g_{pq}}$$

where  $i \neq p \neq q$ , *N* is the number of nodes,  $g_{pq}$  represents the number of the shortest pathways between node *p* and node *k*, and  $n_{pq}^{i}$  represents the number of the shortest pathways containing node *i*.

Closeness centrality ( $C^c$ ): This indicator indicates the topological distance between a node and other nodes in the network, reflecting the overall impact of a node on all other nodes within the network (Wehmuth and Ziviani, 2013). The formula for calculating closeness centrality is given by

$$C_i^c = \frac{N-1}{\sum_{j=1}^N d_{ij}}$$

where  $i \neq j$ , N is the number of nodes, and  $d_{ij}$  is the topological distance from node *i* to node *j*.

### 2.4 Identifying the Technological Solutions

This module focuses on identifying all known and potential technological solutions in the given field—OHSS in our case. Here, multi-component structures are extracted from the heterogeneous knowledge network constructed in Section 2.2 to identify the technological solutions. Multi-component structures are formed by the entities in different technological components as well as the associated connections between these entities. As the heterogeneous knowledge network is generated from data in the scientific papers, this step essentially extracts the solutions hidden in scientific research. The analysis procedure is shown in Figure 4.

It is generally accepted that scientific research provides a fundamental basis for technology-oriented innovations. There are three main layers in the technology-oriented innovation processes: science, technology and industry. Therefore, according to the idea that scientific papers contain important information about future technological developments, two types of technological solutions can be derived by detecting the technology gaps between scientific data and patent data. One is solutions that have already been developed, which we can find in patents. The other is underdeveloped technologies that have some basis in research but have not yet been patented.

The prior art of each patent is identified by calculating and matching keywords in the patent document (See **Figure 5** for calculation process). To begin with, the values of the entities in each component are calculated based on their word vectors, which is the sum of the corresponding word frequency. Then, the entity with the highest word frequency is used to represent the corresponding component. In this way, the technological solution of a patent can be determined. For example, in **Figure 5**, Cn, M1, and F2 are the entities with the highest word frequency among the three technological components respectively, so the final technological solution is Cn-M1-F2.

### 2.5 Evaluating and Predicting the Development Potential of Technological Solutions

To analyze the development potential of these technological solutions and predict which solutions will be the most promising, we established a comprehensive indexing system that measures the utility of each entity. From these figures, we can then calculate the total utility of a technological solution. The indexing system includes six indicators—four indicators for



evaluating the importance of a technology and two indicators for evaluating the potential of a technology. Fuller descriptions of these indicators are given in **Table 1**. With these values calculated, we applied each index to predict the technological innovation opportunities available. To validate our method, we divided the dataset into two parts: Dataset 1

#### **TABLE 2** | Weights of different types of edges.

Туре	Weight	Number	Examples	
C-M	527	122	Hydrogen (C)-Metal-organic framework (M)	
C-F	255	71	2-propanol (C)-Direct fuel cell (F)	
M-F	167	64	Carbon nanomaterials (M)-Proton exchange membrane fuel cell (F)	



covering the period 2008–2017, and Dataset 2 for the period 2018–2019. Dataset 1 was used to derive importance, and Dataset 2 was used to calculate the frequency indicators. The testing procedures are shown in **Figure 6**. First, we used a linear regression to construct the prediction model. Dataset 1 (2008–2017) was used to calculate the value of each indicator, which was taken as the independent variable of the prediction model. Dataset 2 (2018–2019) was used to calculate the frequency of each entity in the technological solutions, which was taken as the dependent variable. Second, the formula for the technology prediction model was derived by a regression analysis and its validity was also verified. Finally, we used all the historical data from 2008 to 2019 to predict the utility value of each

technological entity. Hence, the total utility value of each technological solution was calculated and the most promising future solutions were identified. The results of all these steps are discussed in the next section.

### **3 DATA ANALYSIS AND RESULTS**

### 3.1 The Entities Extracted

We used the Web of Science (WoS) and the Derwent Innovations Index (DII) databases as our data sources. The selected time range for the data was from 2008 to 2019. The search strategy implemented was TS = [((hydrogen storage) OR (solid



storage) OR (onboard storage)) AND ((fuel cell vehicle) OR (fuel cell car) OR (fuel cell bus) OR (fuel cell))]. From this search, 4,039 scientific papers and 3,828 patent documents were retrieved.

The data were cleaned and transformed with the natural language processing tool in the text-mining software VantagePoint. We then assembled a word-frequency list. The 500 most frequently used words were used as our initial sample, and we manually removed the common words that had no specific meaning to OHSS (e.g., gas, fuel cell). We also removed descriptive words that indicated technological performance, such as parameters, qualities, and functions (e.g., 12.1 mm, tensile strength, filling pressure). Thus, 167 keywords were refined from our starting list of 500 high-frequency terms. Next, we merged keywords that had the same meaning. For example, proton exchange membrane fuel cell and polymer electrolyte membrane fuel cell were merged into PEMFC. H2 and hydrogen gas were merged into hydrogen. After these processing steps, 66 unique technological entities remained. We then transformed the unstructured documents into entity frequency vectors and used them to form a  $4,039 \times 66$  scientific document-entity matrix and a  $3,828 \times 66$  patent document-entity matrix. From the document-entity matrices, we selected any document that included two or more entities to result in two filtered datasets.

Next, we used VantagePoint's PCA module to analyze the filtered data, discovering 14 principal factors which covered 65%

of the total terms. **Figure 7** shows the map of these factors, reflecting main technology topics and their relationships. From discussions with domain experts, we extracted three core technological components: hydrogen carrier (C), hydrogen storage material (M), and fuel cell (F), which constitutes the knowledge structure of the OHSS field. Within these components, hydrogen carrier involved 15 technological entities and 39 keywords; hydrogen storage material contained 43 technological entities and 108 keywords; and fuel cell contained 8 technological entities and 20 keywords.

# 3.2 The Heterogeneous Knowledge Network Constructed

We then constructed a weighted heterogeneous knowledge network based on the 66 technological entities (nodes). These entities had 959 edges between them reflecting co-occurrence across nodes at the document-level. According to the technological component each node belonged to, there were three types of edges in total (see Table 2)-527 edges represented hydrogen carrier-hydrogen storage material (C-M) component connections, which is the most frequently occurring connection. The second-most frequently occurring connection was hydrogen carrier-fuel cell (C-F) with 255 edges. And connections between hydrogen storage material-fuel cell (M-F) represented only 167 edges, which is





### TABLE 3 | The OHSS technological solutions for the period 2008–2019.

Technological solutions from 2008 to 2019	Status
Hydrogen—inorganic salts—PEMFC	developed
Hydrogen-complex metal hydrides-PEMFC	developed
Hydrogen-metal hydrides-PEMFC	developed
Hydrogen-metal-organic frameworks-PEMFC	developed
Hydrogen-carbon nanocomposites-PEMFC	developed
Hydrogen-carbon nanomaterials-PEMFC	developed
Hydrogen-liquid organic hydrogen carriers-PEMFC	developed
Hydrogen-inorganic salts-SOFC	developed
Hydrogen-complex metal hydrides-SOFC	underdeveloped
Hydrogen-metal hydrides-SOFC	developed
Hydrogen-metal-organic frameworks-SOFC	underdeveloped
Hydrogen-carbon nanomaterials-SOFC	developed
Hydrogen-liquid organic hydrogen carriers-SOFC	underdeveloped
Hydrogen-inorganic salts-AFC	developed
Hydrogen-metal hydrides-AFC	developed
Hydrogen-carbon nanomaterials-AFC	developed
Methanol-low-temperature liquid phrase-PEMFC	developed
Methanol-low-temperature liquid phrase-SOFC	underdeveloped
Methanol-low-temperature liquid phrase-DFC	developed
Methanol-inorganic salts-PEMFC	developed
Methanol-inorganic salts-DFC	developed
Methanol-inorganic salts-AFC	underdeveloped
Ethanol-low-temperature liquid phrase-PEMFC	developed
Ethanol-low-temperature liquid phrase-SOFC	developed
Ethanol-low-temperature liquid phrase-DFC	developed
Ethanol-low-temperature liquid phrase-AFC	underdeveloped
Ethanol-inorganic salts-PEMFC	developed
Ethanol-inorganic salts-SOFC	underdeveloped
Ethanol-inorganic salts-DFC	developed
Ethanol-inorganic salts-AFC	underdeveloped
Isopropanol-low-temperature liquid phrase-DFC	developed
Isopropanol-inorganic salts-DFC	developed
Urea-low-temperature liquid phrase-SOFC	developed
Urea-low-temperature liquid phrase-DFC	developed
Urea-low-temperature liquid phrase-AFC	underdeveloped
Urea-inorganic salts-PEMFC	developed
Urea-inorganic salts-SOFC	underdeveloped
Urea-inorganic salts-DFC	developed

Note: PEMFC, proton exchange membrane fuel cell; SOFC, solid oxide fuel cell; AFC, alkaline fuel cell; DFC, direct fuel cell.

the lowest frequency. **Table 2** also shows an example of the connections between different components. As can be seen, the connection between hydrogen and metal-organic framework is part of the C—M family of edges. So studies associated with this edge focus on technological solutions that take hydrogen as an energy carrier and a metal-organic framework as a hydrogen storage material.

Now suppose that all the nodes in one component could form a cross-component connection with all the nodes in other components. Then the network would have 1,109 crosscomponent connections. However, the number of connections in the current network is 257, indicating that many potential associations still exist. However, even if the OHSS research were to be quite mature, it is unlikely that every cross-component connection would be formed. It is for this reason that tracing the developments trend of research and identifying the connections that are likely to form is of such great significance to those interested in technology opportunity analysis.

### 3.3 The Dynamics of the Network Revealed

**Figures 8–10** illustrate the heterogeneous knowledge networks of OHSS for the periods 2008–2011, 2012–2015, and 2016–2019, respectively. As can be seen, the overall network density is increasing over time, and this intensification appears to speed up from the second period to the third period. However, from 2012 to 2015, we only see the addition of one more node over the former period. Additionally, several new connections form between the existing nodes. During the period from 2016 to 2019, 18 newly generated nodes were added to the network, and we also see 48 new connections. The total scale of the network grew to 60 nodes and 126 edges. Within this, the highest number of single-node connections grew from 20 during 2008–2011 to 46 during 2016–2019.

In the first period, the research is distributed relatively evenly between each entity, forming a balanced distribution network. No evident research tendency can be seen. However, during the period 2012–2015, we see several core nodes with high centrality emerge. From 2016 to 2019, this trend develops further, and the importance of those core nodes continues to increase. As shown in **Figures 8–10**, aside from hydrogen, two new hydrogen carriers become essential—methanol and urea. Additionally, inorganic salts, metal hydrides, low-temperature liquid phase and metal-organic frameworks become the most commonly used material for hydrogen storage. PEMFCs and solid oxide fuel cells also become the most popular fuel cells in mass application.

Supplementary Appendices SA.1, SA.2, and SA.3 show the top 15 nodes associated with three different centrality measures during the three periods respectively. Comparing these three tables shows us how these core nodes have aggregated, transferred, and disseminated knowledge in the different periods. Further, integrating our analyses of the three centrality measures in Figures 8-10 reveals the main development trends in the network. The results show that the OHSS knowledge network has a star topology, in which all nodes connect to a few core nodes. This forms a radial network pattern with a few nodes as kernels. The most representative technologies are inorganic salts, low-temperature liquid phase, metal-organic frameworks, and liquid organic hydrogen carriers. Research on inorganic salts first appeared during 2008-2011 and was widely put into application in the following two periods. Eventually, it surpassed the popularity of low-temperature liquid phase and metal hydrides, becoming a core technology in the field of hydrogen storage. Moreover, metal organic frameworks becomes more and more central throughout the three periods to the point that it becomes a key core technology in the field during the last period 2016-2019. Liquid organic hydrogen carriers does not appear in the top 15 centralized technological entities in terms of any centrality dimensions in the first two periods. However, it suddenly appears as the top centralized technology from 2016 to 2019. Thus, this promising hydrogen storage technology has become a hot direction of technological innovation. A converse example is found in lowtemperature liquid phase. Although it appeared in the top 15 centrality list during 2012-2015 and 2016-2019, its centrality ranking has declined significantly over time. This combined with



a downward trend in newly formed connections shows that lowtemperature liquid phase has become a relatively inactive research field.

**Figure 11** shows the top 10 weighted edges for the three periods. This chart shows that hydrogen -metal hydrides, hydrogen - PEMFC, hydrogen—NaBH4, and metal hydrides - PEMFC are the most important technology combinations during each period. In addition, since 2012–2015, the weight of hydrogen—metal—organic frameworks has gradually increased, indicating that many studies have been conducted on this technology combination. This is usually a sign that it has great potential for further development.

Turning to the newly emerging nodes and edges during 2016–2019, **Supplementary Appendix SB** presents the top 15 representative entity pairs for further analysis. These technologies have emerged in recent years and corresponding research is relatively limited. Therefore, these technology combinations could be clues as to the technology opportunities and innovations of tomorrow. Technologies such as carbon fiber reinforced plastic, carbon nanofibers, carbon spheres, fullerene, and silicon carbide nanotubes have found new roles in OHSS. Other technologies such as electrospun carbon nanofibers, covalent organic frameworks, and carbon nanocomposites are newly applied in combination with PEMFCs. We believe that these technology combinations provide insights into the future research and innovation trends of OHSS.

### 3.4 The Technological Solutions Identified

Technological solutions are multi-component structures in the knowledge network. As mentioned above, in our knowledge networks, there are three core technological components: hydrogen carriers (C), hydrogen storage materials (M) and fuel cells (F). Therefore, we are primarily interested in technological solutions with a three-component structure;

structures including only one or two technological components were excluded. We found and extracted 38 of these C-M-F chains, i.e., technological solutions, in the networks, as shown in **Table 3**.

The number of patents associated with a technological solution is a simple and effective way to reveal technology opportunities. The higher the number of patents related to technological solutions, the higher the degree of technological development. Among the 38 identified technological solutions, 28 were developed technological solutions. In addition, if a technological solution is associated with research activity but there are no or few corresponding patents, then that technology is underdeveloped and likely holds promise for future development. We identified 10 underdeveloped technological solutions, which have scientific research foundations but with no corresponding patents during the period of study. These are all potential technology opportunities for innovative firms to focus on.

# 4 EVALUATION AND TECHNOLOGY PREDICTION

### 4.1 The Technological Solutions Evaluated

After identifying the developed and underdeveloped technological solutions, the next step is to evaluate the development potential of these technological solutions for technology prediction. Before calculating the utility of the technological solutions, each entity of the technological solution needs to be evaluated. Using a regression analysis, we established a prediction model based on data over the full period of study, 2008 to 2019.

Following the indexing system in outlined in **Section 2.4**, we identified the relationships between the entities and the indicators. First, we took the data for each technological entity from 2008 to 2017 and calculated the value of each indicator as

#### TABLE 4 | Utility levels of 38 technological solutions.

Rank	Technological Solutions	Utility	Status
1	Hydrogen-inorganic salts-SOFC	0.690	developed
2	Hydrogen-carbon nanomaterials-SOFC	0.676	developed
3	Hydrogen – metal hydrides – SOFC	0.667	developed
4	Hydrogen-inorganic salts-PEMFC	0.661	developed
5	Hydrogen-metal-organic frameworks-SOFC	0.652	underdeveloped
6	Hydrogen-carbon nanomaterials-PEMFC	0.647	developed
7	Hydrogen-liquid organic hydrogen carriers-SOFC	0.640	underdeveloped
8	Hydrogen-metal hydrides-PEMFC	0.638	developed
9	Hydrogen-complex metal hydrides-SOFC	0.633	underdeveloped
10	Hydrogen-metal organic frameworks-PEMFC	0.623	developed
11	Hydrogen-inorganic salts-AFC	0.622	developed
12	Hydrogen—carbon nanocomposites—PEMFC	0.611	developed
13	Hydrogen-liquid organic hydrogen carriers-PEMFC	0.611	developed
14	Hydrogen-carbon nanomaterials-AFC	0.608	developed
15	Hydrogen-complex metal hydrides-PEMFC	0.604	developed
16	Hydrogen-metal hydrides-AFC	0.599	developed
17	Methanol-low-temperature liquid phrase-SOFC	0.205	underdeveloped
18	Methanol-inorganic salts-PEMFC	0.185	developed
19	Methanol-low-temperature liquid phrase-PEMFC	0.176	developed
20	Ethanol-inorganic salts-SOFC	0.164	underdeveloped
21	Ethanol-low-temperature liquid phrase-SOFC	0.155	developed
22	Methanol—inorganic salts—DFC	0.151	developed
23	Methanol—inorganic salts—AFC	0.146	underdeveloped
24	Methanol-low-temperature liquid phrase-DFC	0.142	developed
25	Ethanol—inorganic salts—PEMFC	0.135	developed
26	Ethanol-low-temperature liquid phrase-PEMFC	0.126	developed
27	Urea—inorganic salts—SOFC	0.117	underdeveloped
28	Urea-low-temperature liquid phrase-SOFC	0.108	developed
29	Ethanol—inorganic salts—DFC	0.101	developed
30	Ethanol-inorganic salts-AFC	0.096	underdeveloped
31	Ethanol-low-temperature liquid phrase-DFC	0.092	developed
32	Urea—inorganic salts—PEMFC	0.088	developed
33	Ethanol-low-temperature liquid phrase-AFC	0.087	underdeveloped
34	Urea—inorganic salts—DFC	0.054	developed
35	Isopropanol-inorganic salts-DFC	0.054	developed
36	Urea-low-temperature liquid phrase-DFC	0.045	developed
37	Isopropanol-low-temperature liquid phrase-DFC	0.045	developed
38	Urea-low-temperature liquid phrase-AFC	0.040	underdeveloped

**TABLE 5** | The top 10 technological solutions in the conceptual stage.

Rank	Technological solutions	Utility
1	Hydrogen—carbon nanocomposites—SOFC	0.640
2	Hydrogen-metal-organic frameworks-AFC	0.584
3	Hydrogen-carbon nanocomposites-AFC	0.572
4	Hydrogen-liquid organic hydrogen carriers-AFC	0.572
5	Hydrogen-complex metal hydrides-AFC	0.565
6	Methanol-inorganic salts-SOFC	0.214
7	Methanol-low-temperature liquid phrase-AFC	0.137
8	Isopropanol-inorganic salts-SOFC	0.117
9	Isopropanol-low-temperature liquid phrase-SOFC	0.108
10	Isopropanol-inorganic salts-PEMFC	0.088

our independent variables. Then we took the frequency data for each entity during 2018–2019 as the dependent variables. All results were then normalized. The results of this exercise are shown in **Supplementary Appendix SC.1**, and the results of the regression analysis, conducted with SPSS software, are shown in **Supplementary Appendix SC.2**. The regression analysis shows a correlation coefficient R of 0.995, a determination coefficient  $R^2$  of 0.989, and significance at the 0.001 level, which verifies the validity of the proposed model. Consequently, we find a prominent linear correlation between the dependent variable Y and the independent variables I1, I2, I3, I4, P1, and P2. With this regression coefficient, we constructed a utility model as follows:

 $Y = 0.015 - 0.369I_1 + 0.003I_2 + 0.634I_3 + 0.508I_4 - 0.372P_1 + 0.338P_2$ 

## 4.2 The Future Technological Solutions Predicted

To predict future entity utility levels, we used data from the full period (2008–2019). The indicator values are given in **Supplementary Appendix SC.3**, and **Figure 12** shows the values of Y from the above prediction model, which are the future utility levels of each technological entity. The future utility

of the technological solutions are derived by summing the utility levels of each constituent entity. **Table 4** shows the total utility values of 38 published technological solutions, including the 28 developed technological solutions and the 10 underdeveloped technological solutions.

According to Figure 12, we can see that hydrogen, inorganic salts, and SOFC have the highest utility. The technological solution hydrogen-inorganic salts-SOFC has the highest utility, which is verified in Table 4. Among all technological solutions, the top three technological solutions are hydrogen—inorganic salts—SOFC, hydrogen-carbon nanomaterials-SOFC and hydrogen-metal hydrides-SOFC. These developed technological solutions are currently fundamental and mainstream technologies in OHSS. As such, there should be substantial opportunities for further development over the next 2-3 years; however, these opportunities will be coupled with fierce competition. Firms should therefore choose the technological solutions that most suit their needs, capabilities, and development goals and, accordingly, formulate short-term research and development plans.

In terms of underdeveloped technological solutions, the top three technological solutions are hydrogen-metal-organic frameworks—SOFC, hydrogen—liquid organic hydrogen carriers-SOFC, and hydrogen complex metal hydrides-SOFC. As can be seen, the technological solutions that combine the new hydrogen storage material "metal - organic frameworks", "liquid organic hydrogen carriers" and "complex metal hydrides" with the traditional technology combination of "hydrogen and SOFC" are the most prominent and promising future technological solutions. Consequently, in the medium term (4-10 years), firms should focus on these technological solutions.

Additionally, after traversing every possible C-M-F chain in fully connected heterogeneous knowledge network of OHSS, we can exclude some obviously unreasonable technological solutions. For example, hydrogen cannot be stored in a lowtemperature liquid state, and carbon nanomaterials, complex metal hydrides, carbon nanocomposites, and metal organic frameworks are limited to forming technological solutions with hydrogen. There are also several solutions that are still in the conceptual stage and have no real basis in scientific research yet. These are long-term opportunities worthy of investment over the next 10 years, as shown in **Table 5**.

## **5 CONCLUSION AND PROSPECT**

As a power technology with zero carbon emissions, OHSS is an important element of future transportation scenarios and emerging smart grids. Over the last decade, there have been several promising breakthroughs that will take OHSS from an experimental technology to one of mass production with widespread applications. Thus, exploring new technology opportunities in OHSS is of critical importance to researchers, specialists, and enterprise managers. To this end, we developed a novel methodology based on a heterogeneous knowledge network to provide insights into the efforts, knowledge gaps, and dynamics of this thriving field. The methodology begins with scientific papers and patents as the basis for analyzing the technological composition of the field. From this, we built a heterogeneous knowledge network and applied a series of well-designed evaluation indicators that revealed developed and underdeveloped technological solutions over the short-term, medium-term and long-term. Our results with OHSS suggest that the framework is a very effective solution for technology opportunity analysis and prediction.

The main contributions of this study are fourfold: 1) We make a holistic review of scientific and technological evolution in OHSS. 2) We present a novel methodology based on heterogeneous knowledge networks for identifying technological solutions. We applied this methodology to the field of OHSS; however, the methods can be generalized to any scientific field. 3) We offer an evaluation and prediction model for generating more accurate predictions of the potential within a technological solution. 4) We provide a comprehensive technology opportunity analysis of the field of OHSS.

Our analysis of OHSS identified three core technological components, including 66 technological entities, among which metal hydrides, inorganic salts, low-temperature liquid phrase and metal-organic frameworks are the most significant hydrogen storage materials at present. Of these, liquid organic hydrogen carriers are the fastest growing emerging hydrogen storage material in recent years. The fuel cell technologies that received the most attention are PEMFCs and SOFCs. PEMFCs have a stronger development momentum and are leading to intense competition. Methanol and ethanol are considered to be extremely efficient hydrogen carriers with tremendous growth potential in the future. In addition, other hydrogen sources, such as isopropanol and urea, also shows good application prospects for hydrogen storage.

We also identified 38 technological solutions, of which 28 are developed and 10 are underdeveloped. In the short-term, the solutions with the highest combined utility value are the ideal technology selections, such as hydrogen-inorganic salts-SOFC, hydrogen-carbon nanomaterials-SOFC and hydrogen-metal hydrides-SOFC. The underdeveloped technological solutions, which have relatively high utility level but are still in the stage of fundamental research are medium-term prospects for enterprise planning. These solutions include hydrogen-metal-organic frameworks-SOFC, hydrogen-liquid organic hydrogen hydrogen carriers—SOFC and \_ complex metal hydrides-SOFC. Solutions with little to no basic research and that have not been developed in practice are long-term technology directions with great R&D potential. These solutions include hydrogen-carbon nanocomposites-SOFC, hydrogen-metal-organic frameworks—AFC and hydrogen-carbon nanocomposites-AFC.

This study focuses on understanding the technological knowledge of OHSS. The results present some common technological entities associated with OHSS, but, through association analysis, they also reveal some new findings about the possible innovation pathways of OHSS. Hence, from one perspective, the proposed methodology can be seen as a tool for seeking technological solutions from existing OHSS research. Yet, from another perspective, it can be used a decision support system that produces insights into technology trends and potential directions of development that can help to create cutting-edge technologies, optimize business strategies, and maximize profits.

However, as with all studies, our has some limitations and future development work that needs to be considered. First, these results should be interpreted with caution, as we assumed that technological innovations mainly originate from the recombination of existing heterogeneous technological knowledge. The assumption that new technologies and ideas strictly emerge on the basis of old technologies could lead to biased outcomes, as many technologies are disruptive technologies or mutational technologies which may not stem from previous themes. To enhance the efficiency and practicality of the proposed methodology, some additional quantitative measures could be considered. Second, there are other important data sources, such as project data, product data, and market data that can contribute to further knowledge discovery activities. Thus, integrating additional data sources into the proposed methodology could generate a more reliable picture of future technological innovation. Third, although we can effectively forecast future technological solutions based on the proposed evaluation index system, the corresponding indexes could be further improved. Future research might take into account technical performance and technical risk. Finally, the results presented in this research may be limited because the research focuses on a single technology field. In the future, we plan to apply the proposed methodology to other fields to check its robustness.

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### DATA AVAILABILITY STATEMENT

The raw data supporting the conclusion of this article will be made available by the authors, without undue reservation.

### **AUTHOR CONTRIBUTIONS**

XS: conceptualization, methodology, experimental investigation, software, and original draft preparation. LC: validation, data curation, visualization, and reviewing and editing. ZL and YC: read and supervision. All authors provided critical feedback and helped shape the research, analysis and manuscript.

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### SUPPLEMENTARY MATERIAL

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