



# Generating novel research ideas using computational intelligence: A case study involving fuel cells and ammonia synthesis



Takaya Ogawa\*, Yuya Kajikawa

Graduate School of Innovation Management, Tokyo Institute of Technology, 3-3-6 Shibaura, Minato-ku, Tokyo 108-0023, Japan

## ARTICLE INFO

### Keywords:

R & D management  
Bibliometrics  
Keyword similarity  
Ammonia synthesis  
Fuel cell

## ABSTRACT

We proposed a method to help researchers create novel research ideas using bibliometrics. Different concepts and techniques exist in different research areas, and when the fields are sufficiently similar, a salient combination of two different areas can lead to the development of novel research. We have assumed that two different research areas, sharing a high number of similar keywords, would be excellent candidates for integration. We combined link mining and text mining techniques to elucidate hidden but implicit opportunities among apparent, explicit research clusters. To demonstrate the effectiveness of our approach, we conducted a case study on fuel cells and ammonia synthesis. Fuel cells are a rapidly growing research field, while ammonia synthesis is relatively mature. Our results successfully extracted a plausible and post-mature research idea.

## 1. Introduction

Ideas for new and original products, services, systems, and techniques generally derive from the human ability to imagine, design, and invent. Impressive original works that result in the creation of value are regarded as innovation. Innovation, the key to much human activity and societal advancement, is expected to promote development and to resolve both overt and latent social problems. In addition to the enthusiastic experimentation of practitioners, this method for achieving innovation has been theoretically and empirically studied in academia. However, as we know well, no formula or formal methodology can guarantee innovation. Academic research does not generally support innovation because it focuses on understanding how innovation occurs from a scientific point of view rather than on using engineering and design to innovate. The recent development of computational intelligence offers new ways to support intelligent human invention and innovation. Computational creation and the support of salient and innovative ideas constitute a great challenge; they can help to empower human beings and develop society.

Among myriad methods for creating innovation, one possible approach is to combine different types of knowledge (Schumpeter, 1934). The combination, integration, and fusion of different areas of expertise can generate a seed of original knowledge (Swanson, 1986). Human activity often involves collaboration as people combine knowledge to uncover novel insights (Katz and Martin, 1997). However, the extent of accumulated human knowledge is so huge that no one researcher can make use of it all (Kajikawa et al., 2006). There must

therefore be many undetected combinations of knowledge with the potential to produce innovations.

The field of bibliometrics has recently been developed to overcome the above difficulty. In bibliometrics, citation network analysis is being used effectively to identify emerging academic research clusters and to analyze their characteristics without the need to review individual papers. For example, citation network analysis has been used to confirm the rapid growth of fuel cell and solar cell technology research in the field of energy research (Kajikawa et al., 2008). Ho et al. have applied citation network analysis to research trends and the development path of fuel cell technology (Ho et al., 2014). Citation network analysis has also been used to identify mutually influential biofuel research topics (Kajikawa and Takeda, 2008). Other researchers have used journal citation data and journal classification data to describe the network of energy-related journals (Dalpe and Anderson, 1995; Tijssen, 1992). In addition to network analysis, text analysis is used to assess multi-word phrase frequencies and phrase proximities, and to extract the taxonomic structure of energy research (Kostoff et al., 2002, 2005).

The existing literature on bibliometrics tends to focus on describing the overall structure and trend of a selected research domain using either text or citation analysis. Recently, the combined use of citation network and text analysis has been developed; this computational method can reveal linkages between two research areas using publication data. Citation network analysis is a powerful tool for illuminating the explicit relationships among papers, while text analysis can be used to extract implicit relationships. After extracting citation clusters based on explicit data (i.e., citations), text analysis can be applied to extract

\* Corresponding author.

E-mail addresses: [takaya.o.aa@m.titech.ac.jp](mailto:takaya.o.aa@m.titech.ac.jp) (T. Ogawa), [kajikawa@mot.titech.ac.jp](mailto:kajikawa@mot.titech.ac.jp) (Y. Kajikawa).

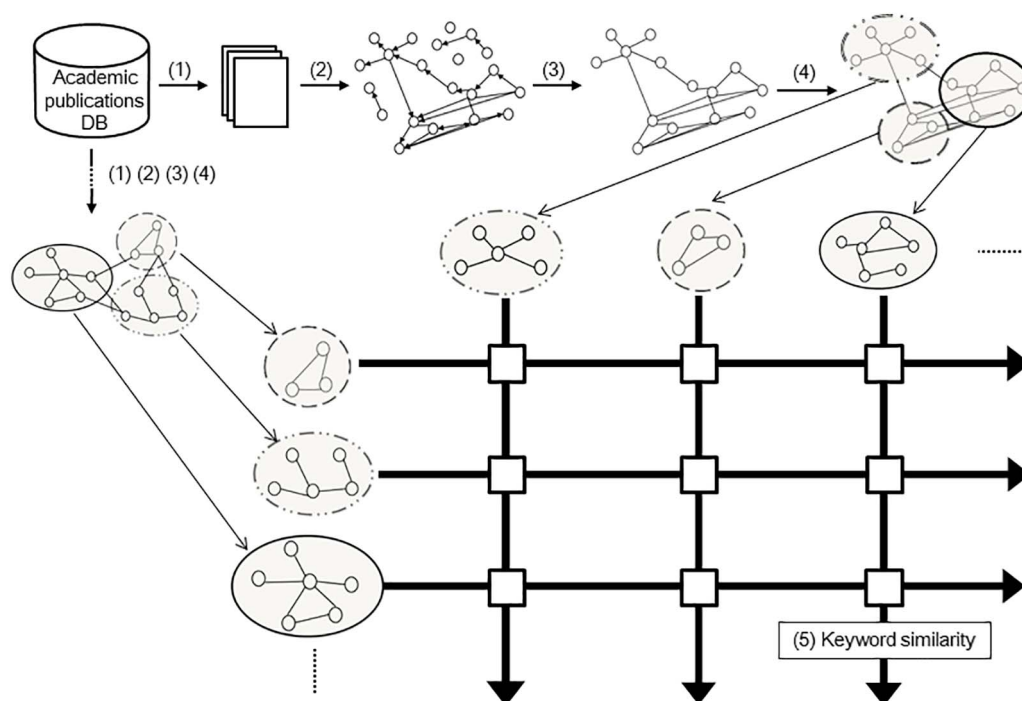


Fig. 1. Schematic illustration of clustering and measurement using keyword similarity.

the hidden relationships that do not appear in the citation information. For example, Shibata et al. compared structures related to the citation network of scientific publications with those of patents in solar cell research and discussed whether linkages existed, revealing academic research areas that were not yet commercialized (Naoki Shibata and Sakata, 2010). Ogawa et al. analyzed research elements with commercial potential in areas related to polymer electrolyte fuel cells (Ogawa and Kajikawa, 2015). They used network analysis to divide academic research papers into research clusters, measuring “patent relatedness” by using textual similarities between the research cluster and existing patents. Nakamura et al. highlighted unexplored areas, including water use in the aviation industry, which was detected by combining the citation and text analysis of environmental and aviation industry issues (Nakamura et al., 2014). In the same way, Vitavin et al. succeeded in finding links between robotics and gerontology, leading to the development of new ways to use robots to help elderly people (Ittipanuvat et al., 2014).

In this study, we applied the computational method to create a novel research idea by combining knowledge drawn from two different research areas using network analysis and keyword similarity. We assumed that recent areas of research have a lot of novel technologies and will eventually develop into traditional research areas. For the recent research area, the computational method was applied to the fuel cell, which is a highly energy-efficient device that was developed recently. The traditional research area was ammonia synthesis, an extremely important process that has changed very little during the past 100 years and still relies on the Haber-Bosch process, which requires very high pressure and temperatures. The final goal of this research was to develop a new approach that can revitalize the traditional research area of ammonia synthesis by applying the latest fuel cell techniques. Bibliometric data from both research areas were divided into several clusters (focusing on each individual technology) using network analysis. The divided clusters of one area were compared with clusters from the other research area using keyword similarity so that areas of relatedness could be identified. A high level of keyword similarity between clusters suggested that techniques used in those clusters could be shared. In the next section, we will provide illustrations of the methodology adopted in this paper.

## 2. Data and method

### 2.1. Data

We collected bibliographic data from academic publications on fuel cells and ammonia synthesis. Data from these academic papers, including the title, author, publication year, abstract, address, and references, were retrieved from the Science Citation Index Expanded (SCI-EXPANDED), compiled by the Thomson Reuters Institute for Scientific Information (ISI). We used the query “fuel cell\*” to collect data on fuel cells. In the case of ammonia synthesis, we used a rather complex query to identify and recall relevant papers. The query was as follows: “ammonia synthesis\*” or “synthesis\* of ammonia” or “ammonia formation\*” or “formation\* of ammonia” or “NH<sub>3</sub> formation\*” or “formation\* of NH<sub>3</sub>” or “nitrogen protonation\*” or “protonation\* of nitrogen” or “N<sub>2</sub> protonation\*” or “protonation\* of N<sub>2</sub>” or “NH<sub>3</sub> synthesis\*” or “synthesis\* of NH<sub>3</sub>” or (“nitrogen fixation\*” or “fixation\* of nitrogen”) and (“ammonia” or “NH<sub>3</sub>”) or (“N<sub>2</sub> fixation\*” or “fixation\* of N<sub>2</sub>”) and (“ammonia” or “NH<sub>3</sub>”) or “synthetic\* ammonia” or “synthetic\* of ammonia” or “synthetic\* NH<sub>3</sub>” or “synthetic\* of NH<sub>3</sub>” or “ammonia synthetic process\*” or “synthetic process\* of ammonia” or “NH<sub>3</sub> synthetic process\*” or “synthetic process\* of NH<sub>3</sub>” or “ammonia production\*” or “production\* of ammonia” or “NH<sub>3</sub> production\*” or “production\* of NH<sub>3</sub>.” The query terms were determined using the following procedure. First, “ammonia synthesis\*” and “synthesis\* of ammonia” were used to collect papers. Then, we read the collected papers and added terms such as ammonia formation, N<sub>2</sub> fixation, and synthetic ammonia. Papers were collected again using the new query; we read them and searched for other terms. We repeated this process until an additional term did not increase the total number of papers by more than 100 over the number collected without the additional term. Data collection was carried out in December 2012.

### 2.2. Method

Our analytical procedure is schematically shown in Fig. 1. In Step (1), the data from academic papers were downloaded. In Step (2), we constructed citation networks by treating the papers as nodes and the

intercitations as links. The network created in each year facilitated a time-series analysis of the citation networks. According to a previous study, intercitation, which is also known as direct citation, is the best-tested approach for detecting emerging trends (Shibata et al., 2009). In network analysis, only the data for the largest graph component were used; we eliminated data not linked to any other papers in Step (3). After extracting the largest connected component, in Step (4) the network was divided into clusters using the topological clustering method of Newman's algorithm, which extracts tightly knit groups of nodes (Newman, 2004). Newman's algorithm employs the following equation:

$$Q = \sum_{s=1}^M \left[ \frac{l_s}{l} - \left( \frac{d_s}{2l} \right)^2 \right], \quad (1)$$

where  $Q$  is the independence of the module,  $M$  is the number of clusters,  $s$  is the cluster,  $l$  is the number of links in the whole network,  $l_s$  is the number of links between both nodes within cluster  $s$ , and  $d_s$  is the sum of the links of the nodes in cluster  $s$ . In Newman's algorithm, the clusters are divided into subgroups to maximize  $Q$ . Eq. (1) is “the probability that reference links exist within clusters” minus “the probability of random links.” This algorithm identifies well-separated clusters in the research area. It is a method that has been used in many research fields, successfully obtaining clusters separated into particular research fields (Kajikawa et al., 2008; Ho et al., 2014; Kajikawa and Takeda, 2008; Small, 2006; Naoki Shibata and Sakata, 2011). These four steps were applied to publication data in both research areas.

Finally, in Step (5), keyword similarity was calculated for each cluster in both research areas. The calculation of keyword similarity was carried out based on the cosine similarity of the term frequency-inverse document frequency (tfidf) vector, which is the best-tested approach for discovering corresponding relationships between two different clusters (Shibata et al., 2011). Eq. (2) of the cosine similarity,  $Cosine(f, a)$ , between clusters focusing on fuel cell  $f$  and ammonia synthesis  $a$  is defined using the term frequency weighting factor,  $FreW$ , as

$$Cosine(f, a) = \frac{\sum \overrightarrow{FreW_{fi}} \times \overrightarrow{FreW_{ai}}}{\sqrt{(\sum \overrightarrow{FreW_{fi}})^2} \sqrt{(\sum \overrightarrow{FreW_{ai}})^2}}, \quad (2)$$

where

$$FreW_{fi} = \frac{n_{fi}}{n_f} \times \log\left(\frac{N_f}{N_{fi}}\right), \quad \text{and} \quad (3)$$

$$FreW_{ai} = \frac{n_{ai}}{n_a} \times \log\left(\frac{N_a}{N_{ai}}\right). \quad (4)$$

$i$  is the term, and  $n_{fi}$  and  $n_{ai}$  are the numbers of occurrences of term  $i$  in clusters  $f$  and  $a$ , respectively.  $n_f$  and  $n_a$  are the total numbers of terms in clusters  $f$  and  $a$ , respectively.  $N_f$  and  $N_a$  are the total numbers of clusters in the dataset of  $f$  and  $a$ , respectively.  $N_{fi}$  and  $N_{ai}$  are the numbers of clusters containing term  $i$  in clusters  $f$  or  $a$ . In calculating keyword similarity, we employed keywords ranked within the top 30 in terms of tfidf.

### 3. Results

#### 3.1. Focused clusters

The number of publications on fuel cells and ammonia synthesis totaled 57,715 and 4682, respectively. Data were divided into 104 fuel cell clusters and 31 ammonia synthesis clusters. Before calculating keyword similarity, we carried out a first trial on major clusters that included a large quantity of papers in order to test the method; we excluded minor clusters that included only a few publications. The focused clusters on fuel cell technologies were the top four, ranked by

the number of publications. They comprised the solid oxide fuel cell cluster (SOFC, 18,253 papers), the catalyst for polymer electrolyte fuel cell cluster (PEFC, 14,788 papers), the electrolyte membrane for PEFC cluster (12,652 papers), and the bio fuel cell cluster (Bio-FC, 3154 papers). Clusters with fewer than 10,000 published papers were excluded. The focused clusters on ammonia synthesis were the top four clusters, ranked by the number of publications. They comprised the cluster relating to the iron catalyst promoted by potassium (559 papers), the cluster relating to the ruthenium catalyst promoted by alkali metal and supported by carbon (530 papers), the artificial ammonia synthesis in moderate conditions cluster (337 papers), and the biological nitrogen fixation cluster (109 papers). Clusters with fewer than 100 papers were excluded.

#### 3.2. Brief explanation of focused clusters

##### 3.2.1. Fuel cell technologies

A fuel cell is an efficient electricity generator that uses a chemical energy source (fuel) such as hydrogen. The entire reaction occurs between fuel and oxygen from air, in which the energy difference of reactants and products is converted into electrical energy. The main components are the catalyst and electrolyte (see Fig. 2, “Schematic image of PEFC,” as representative). The catalyst, which facilitates reactions, is deposited on the electrode, or the catalyst itself is used as the electrode. There are two electrodes: anode (extracting electron) and cathode (receiving electron). The extracted electron works through an electronic device, and the ion that separates from the fuel conducts through the electrolyte to form an electric circuit. The electrolyte also plays the role of separating anode and cathode in order to not mix fuel and product (waste).

In PEFC, the anode extracts the electron from hydrogen and generates  $H^+$ .  $H^+$  is conducted through the electrolyte and reacts with oxygen at the cathode. The best-known proton-conducting electrolyte is Nafion. Generally, platinum is dispersed on carbon as a catalyst (Pt/C) and utilized for both the anode and cathode. A PEFC device employs a catalyst layer in the anode and cathode, which is fabricated by mixing Pt/C and polymer electrolyte (usually Nafion). If the electrode is composed simply of Pt/C, Pt, apart from Nafion, is utilized as  $H^+$  cannot reach the Pt/C (Fig. 3a). In contrast, Nafion in a catalyst layer can convey  $H^+$  to Pt dispersed in the catalyst layer (Fig. 3b). Therefore, a catalyst layer effectively utilizes Pt/C and enhances the activity per electrolyte area. The operating temperature is  $\sim 100^\circ C$ , thus enabling a quick start and stop. It is applied for household electricity generation as well as an energy source for automobiles. A direct methanol fuel cell (DMFC), in which methanol is used as fuel instead of hydrogen, is similar to PEFC. DMFC technologies are included in PEFC clusters.

In SOFC, the cathode donates an electron to oxygen and forms  $O^{2-}$ .  $O^{2-}$  percolates through the electrolyte and reacts with fuel at the anode, passing the electron to the anode. SOFC operates at a much higher temperature of  $700\text{--}1100^\circ C$  as  $O^{2-}$  conductivity is not sufficient at

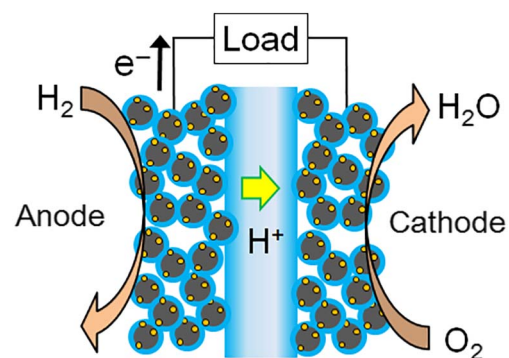


Fig. 2. Schematic image of PEFC. (For interpretation of the references to colour in the text regarding this figure, the reader is referred to the web version of this article.)

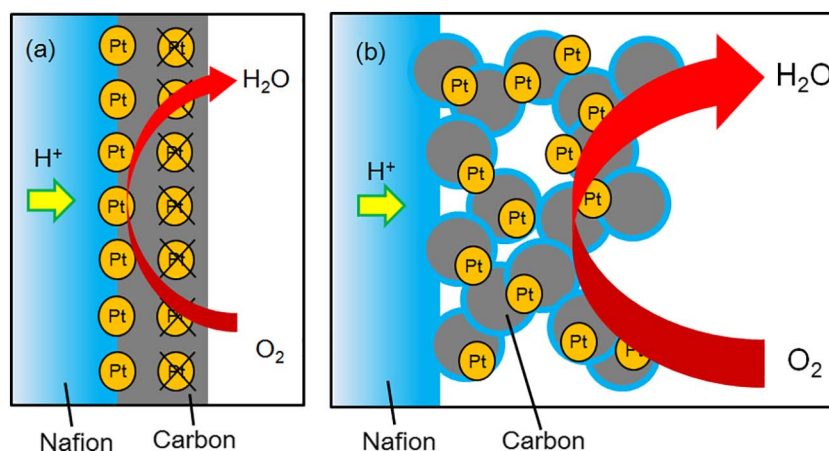


Fig. 3. Schematic image of an electrode without (a) and with (b) a catalyst layer in PEFC.

lower temperatures. The merits of SOFC include high energy efficiency and the low cost of the components and system. The high temperature promotes reaction without the need of expensive metals such as platinum. However, the high operating temperature also imposes slow start-up and shut-down. Hence, SOFC is suitable for large-scale electricity generation with steady operation, which does not require starting and stopping.

A Bio-FC is a fuel cell that generates electricity from sugars such as glucose using an enzyme as a catalyst. The conducting ion is  $H^+$ , and the product is water. Therefore, a Bio-FC can be utilized as an intravital energy source (e.g., an energy source for a heart pacer).

### 3.2.2. Ammonia synthesis

In industry, ammonia is mainly synthesized through the Haber-Bosch process under harsh conditions (400–600 °C and 20–40 MPa) using a heterogeneous iron-based catalyst. The iron-based catalyst is very stable and cheap, and has enough activity, especially when a promoter such as potassium is added to the catalyst. It has, therefore, been the best catalyst for ammonia synthesis in industry for a long time. In the Haber-Bosch process,  $N_2$  dissociates in the adsorption step and forms N. N reacts with H, which dissociates from dihydrogen ( $H_2$ ) in the same way over the catalyst surface. The cluster “iron catalyst promoted by potassium” is related to this traditional process.

Since the 1970s, ruthenium has been a focus of attention as the active heterogeneous catalyst for ammonia synthesis. Ruthenium can produce ammonia under much milder conditions than iron-based catalysts, although the reaction mechanism is the same as in the Haber-Bosch process. However, ruthenium is expensive and has a fatal defect in that it loses activity under high hydrogen pressure. This is because hydrogen can disturb nitrogen adsorption over the ruthenium surface, which is known as hydrogen poisoning. An elevated pressure is thermodynamically favorable and industrially efficient as the ammonia produced can be collected as a liquid. Some promoters (alkali metals) can alleviate hydrogen poisoning, and many studies have investigated several promoters. The cluster “ruthenium catalyst promoted by alkali metal and supported by carbon” focuses on these studies.

Unlike the Haber-Bosch process, enzymes such as nitrogenase can synthesize ammonia at room temperature and atmospheric pressure. The synthesis mechanism is different from Haber-Bosch; in nitrogenase, dinitrogen ( $N_2$ ) reacts with protons ( $H^+$ ) and electrons ( $e^-$ ) one by one and eventually becomes ammonia ( $NH_3$ ). However, the details of the synthesis mechanism over the catalytic center are still unknown. “Biological nitrogen fixation cluster” is the cluster concerning nitrogenase with generic approaches.

Ammonia synthesis under mild conditions, such as at room temperature and atmospheric pressure, is prominent in simplifying the process, resulting in a reduction of ammonia costs. Therefore, many

studies have attempted to imitate nitrogenase artificially; thus, the reaction mechanism is the same as in nitrogenase. One approach involves organometallics (homogeneous catalyst), which produce ammonia using a reducing agent and proton source. Currently, this type of catalyst is fragile, and reactivity is not sufficient. The other approach uses electrochemical synthesis (Fig. 4). Electricity is utilized to reduce nitrogen species and promote the reaction between the species and proton. The “artificial ammonia synthesis in moderate conditions cluster” is related to these.

### 3.3. Keyword similarity

The matrix of keyword similarities between clusters in fuel cell and ammonia synthesis is shown in Table 1. Eight pairs of clusters had a zero similarity value among the 16 clusters, suggesting that techniques could not be usefully shared. Another eight pairs had very different, positive values. In this paper, we focused on the four pairs with high keyword similarities when considering the possibility of combining technologies, as discussed in the following section.

## 4. Discussion

### 4.1. The validity of keyword similarity analysis

Before discussing the novel research ideas produced by combining distant research areas, we can confirm the validity of the similarity measures used. The similarities had a reasonable tendency, as explained below. The main focus was on the materials utilized in each cluster as materials can determine operating conditions and approaches to studies.

We first focused on the “SOFC” column in Table 1, which includes the following: “ruthenium catalyst promoted by alkali metal and supported by carbon,” > “iron catalyst promoted by potassium,” > “artificial ammonia synthesis at moderate condition,” and “biological nitrogen fixation.” The SOFC device operates at a much higher temperature of 700–1100 °C; the component of SOFC is inorganic and stable at such temperatures, unlike organic components in a biological

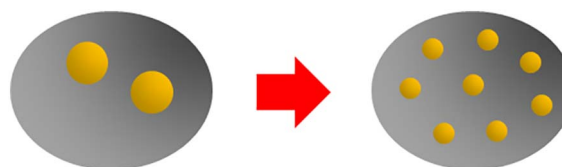


Fig. 4. Schematic image of a dispersed catalyst on carbon: the catalyst is yellow and the carbon is grey. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

**Table 1**  
Keyword similarity matrix between clusters, focusing on ammonia synthesis and fuel cell technology.

Ammonia synthesis/fuel cell	SOFC	Catalyst for PEFC	Electrolyte membrane for PEFC	Bio-FC
Iron catalyst promoted by potassium	0.0403	0.1723	0.0	0.0
Ruthenium catalyst promoted by alkali metal and supported by carbon	0.0447	0.3257	0.0	0.0
Artificial ammonia synthesis in moderate conditions	0.0166	0.0574	0.0746	0.0
Biological nitrogen fixation	0.0	0.0	0.0	0.0249

system. It can therefore be seen that the components in the “biological nitrogen fixation” research cluster (such as enzymes) have nothing in common with components in the “SOFC” cluster; this creates a zero-value similarity between the “SOFC” and “biological nitrogen fixation” clusters. The “artificial ammonia synthesis in moderate conditions” cluster includes research on electrochemical ammonia synthesis at atmospheric (moderate) pressure but high temperatures. The similarity between “artificial ammonia synthesis in moderate conditions” is therefore slightly higher than for “biological nitrogen fixation,” although the basic component includes fragile materials such as organometallics as well as the harsh conditions required for SOFC. At the same time, clusters involving the “iron catalyst promoted by potassium” and “ruthenium catalyst promoted by alkali” both focus on the catalyst used in a Haber-Bosch or similar process—that is, under conditions of high temperature and high pressure. Their components are all inorganics, except for simple carbon (simple carbon is stable without oxygen).

Second, we focused on the “Bio-FC” column. Bio-FC is an energy device operated under moderate conditions and almost the same as a biological system, using an enzyme as a catalyst. The order of similarity (“biological nitrogen fixation” > “artificial ammonia synthesis in moderate conditions” = “ruthenium catalyst promoted by alkali metal and supported by carbon” = “iron catalyst promoted by potassium”) is reasonable, as explained below. As previously mentioned, the components used in the “iron catalyst promoted by potassium” and “ruthenium catalyst promoted by alkali” clusters are very different from biological materials. The cluster involving “artificial ammonia synthesis in moderate conditions” deals with catalysts, including organometallics, which are derived from organic materials. However, the research involved uses conditions (such as the application of voltage) that are remote from biological systems. For this reason, their similarity values are zero. Both the “Bio-FC” and “biological nitrogen fixation” clusters use enzymes as catalysts; for this reason, “biological nitrogen fixation” has the only positive value in this column.

As discussed above, the positive case is reasonable. We can also confirm the other four cells with zero values. In the “biological nitrogen fixation” category, the keyword similarities for “catalyst for PEFC” and “electrolyte membrane for PEFC” are zero. The operating condition of PEFC differs from the conditions for biology; it involves relatively harsh conditions (around 100 °C) and the application of voltage. The catalyst for PEFC is inorganic. The electrolyte membrane is proton-conducting polymer, which is different from an enzyme. Thus, zero values are reasonable. In the “electrolyte membrane for PEFC” column, the keyword similarities for “iron catalyst promoted by potassium” and “ruthenium catalyst promoted by alkali metal and supported by carbon” are zero. Polymer (the PEFC electrolyte membrane) does not exist in the Haber-Bosch process (“iron catalyst promoted by potassium” and “ruthenium catalyst promoted by alkali metal and supported by carbon”). Therefore, these zero-similarity values are also reasonable.

As examined in detail in the following section, the remaining four cells have a high affinity for the interaction of techniques. For this reason, their high values are also reasonable. Based on these results, we concluded that a high keyword similarity value indicates the existence of common material, techniques, and experimental conditions.

#### 4.2. Common techniques associated with high keyword similarity

In this section, we focus on research areas with high keyword similarities in Table 1—namely, “catalyst for PEFC”/“iron catalyst promoted by potassium” (keyword similarity = 0.3257); “catalyst for PEFC”/“ruthenium catalyst promoted by alkali metal and supported by carbon” (keyword similarity = 0.1723); “electrolyte membrane for PEFC”/“artificial ammonia synthesis in moderate conditions” (keyword similarity = 0.0746); and “catalyst for PEFC”/“artificial ammonia synthesis in moderate conditions” (keyword similarity = 0.0574). These high-level keyword similarities should be derived using similar techniques in each research cluster. In the following section, we discuss plausible common research ideas combining fuel cells and ammonia synthesis.

The two previously mentioned combinations—“catalyst for PEFC”/“iron catalyst promoted by potassium” and “catalyst for PEFC”/“ruthenium catalyst promoted by alkali metal and supported by carbon”—have a common characteristic. Regarding ammonia synthesis, they focus on iron or ruthenium supported by catalyst supports such as carbon particles with promoters. Catalyst support is used to finely disperse the catalyst metal in order to process a wide surface area; the surface area is generally important when using a heterogeneous catalyst as reaction occurs on the catalyst surface. A refined catalyst metal on a wide surface area results in high reactivity with the same catalyst volume, resulting in an efficient, low-cost use of the catalyst. For example, if we assume the catalyst is spherical, a half radius of the catalyst leads to a surface area that is two times larger than that of the original radius (Fig. 5). Catalyst support is important for preventing catalysts from coming into contact with each other and aggregating. In addition, alkali metal such as potassium is generally electron-donating and works as a promoter in ammonia synthesis. They enhance catalytic activity through the electron transferred to the catalyst when promoters are deposited near or on the catalyst surface, while promoters isolated from the catalyst contribute less to activity (Fig. 6a). The enriched electron density of the catalyst prompts interaction between the catalyst and dinitrogen, which facilitates the rate-determining step of ammonia synthesis:  $N_2$  dissociative adsorption. Therefore, the catalysts for ammonia synthesis are usually supported and have electron

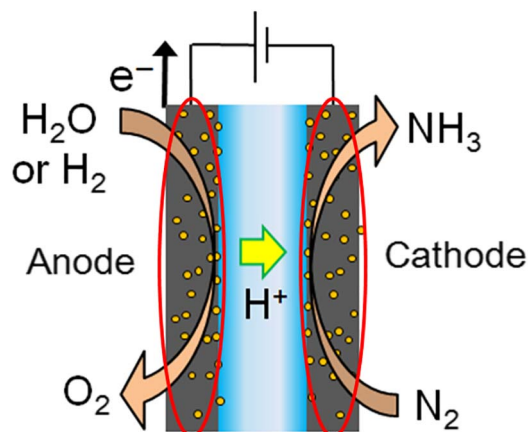


Fig. 5. Schematic image of the electrochemical synthesis of ammonia.

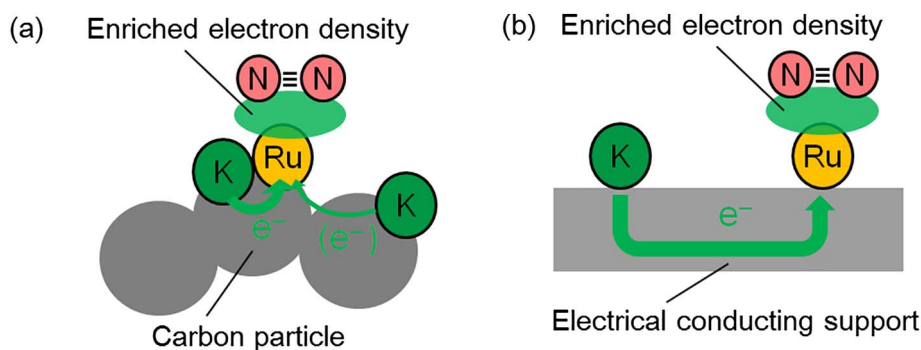


Fig. 6. Schematic image of electron transfer to a catalyst (a) from promoters near the catalyst, and (b) from isolated promoters via electron conducting support (the representative promoter and catalyst are potassium and ruthenium, respectively).

promoters added. In some cases, catalyst support enhances the catalytic activity of the metal by donating electrons from electron-donating support. Moreover, good electrical conductivity of support can contribute to catalytic activity as the isolated electrons of promoters, which do not contact the catalyst, can be effectively passed to the catalyst via electron-conducting support (Fig. 6b; unintentionally, promoters sometimes stay on support without contacting the catalyst).

As for PEFC, carbon provides suitable catalyst support because it is easy to reduce carbon to nano-sized particles spread out across a wide surface area. Moreover, carbon has chemical stability and is low cost. Likewise, in ammonia synthesis research, carbon is readily broken down and distributed across a wide surface area. Hence, these research areas have a common purpose: to finely disperse a catalyst. Thus, these research areas must be interactive so that new techniques being used in fuel cell research can be applied to ammonia synthesis. For example, the technique for dispersing metals on carbon nanotubes and graphene is being keenly studied in the fuel cell research area. Graphene and carbon nanotubes are dimensionally ordered rather than carbon particle, which can lead to a faster mass transfer of reactants and products (Zheng et al., 2012). Furthermore, the electrical conductivity of graphene and carbon nanotubes is much greater than that of carbon particles, facilitating the electron transfer from isolated promoters (Zheng et al., 2012; Saadatjou et al., 2015). These properties will enhance catalytic activity. In particular, nitrogen- or boron-doped graphene and carbon nanotubes are studied as metal-free catalysts in PEFC (Zheng et al., 2012). While nitrogen-dope is electron-withdrawing, boron-dope is electron-donating against carbon. Therefore, boron-doped graphene and carbon nanotubes have the potential to enhance catalytic activity for ammonia synthesis by donating electrons to the catalyst. By simply retrieving SCI-EXPANDED papers, we can access 3066 and 487 papers on carbon nanotubes and graphene, respectively, all published in or before 2012. In the area of ammonia synthesis, only 63 papers on carbon nanotubes and 4 papers on graphene were published before 2012. The techniques for using these nano-carbon materials, developed in the area of fuel cell research, have the potential to greatly improve the dispersion and performance of catalysts in ammonia synthesis.

In the same way, studies of the “electrolyte membrane for PEFC”/“artificial ammonia synthesis in moderate conditions” and the “catalyst for PEFC”/“artificial ammonia synthesis in moderate conditions,” involve potentially interactive research. In the research area of electrochemical ammonia synthesis involved in the cluster “artificial ammonia synthesis in moderate conditions,” nitrogen and hydrogen gas (or water) are separated by a proton-conducting electrolyte such as Nafion. The protons percolate through electrolytes, where electrical force reacts with nitrogen to produce ammonia (Fig. 4). Meanwhile, in the PEFC system, the protons percolate through the electrolyte and react with oxygen in a cathode, generating energy (Fig. 2). As seen in Figs. 2 and 4, the areas covered by this research are very similar, suggesting that the techniques used must be interactive. There are only

around 100 publications on the electrochemical synthesis of ammonia. The potential for using PEFC techniques to develop this area can be expected to be high. Electrochemical ammonia synthesis is promising because ammonia can be synthesized under moderate conditions, such as atmospheric pressure, which results in a simplification of the process. In particular, if ammonia is directly synthesized from water as a hydrogen source, the process of evolving hydrogen from water can be skipped. This can reduce the cost of ammonia.

Recent publications provided by the Tao group demonstrate the application of PEFC techniques to electrochemical ammonia synthesis (Lan et al., 2013). They used commercialized materials such as Nafion and platinum catalyst supported by carbon (Pt/C) for the PEFC. Moreover, a catalyst layer has been applied to ammonia synthesis (Fig. 3b). In order to fabricate the catalyst layer, Nafion was added to a solution of Pt/C, as described in the Methods sections of their papers. The added Nafion allowed protons to reach Pt in the distance between the Nafion separating anode and cathode (the yellow arrow in Fig. 2). In previous electrochemical ammonia synthesis studies, a catalyst layer was not used, and most of the catalyst (the red-circled area in Fig. 4) did not contribute to the reaction (Kordali et al., 1673; Xu and Liu, 2009). As a result of these optimized techniques in PEFC, the reaction rate was much higher, achieving ammonia synthesis using room-temperature water and atmospheric pressure. It has therefore been demonstrated that PEFC techniques can improve research on electrochemical ammonia synthesis. Furthermore, many optimized PEFC techniques, such as measurement techniques and the configuration of a cell electrode, should be shared.

#### 4.3. Research limitations: a balance between recall and precision

In this paper, we have discussed the validity and effectiveness of our approach—namely, identifying common research areas in selected pairs of research clusters to generate novel research ideas. However, we must note the limitations of our research. In addition to selecting pairs of clusters, this project used focused keywords—those listed among the top 30 using tfidf—to compensate for the trade-off problem known as “recall and precision.” When keyword similarity is calculated using not only whole keywords but all of the words that characterize the cluster, the search will include general terms such as “using,” “result,” and “study,” creating noise in the results, which will have high recall but low precision. To obtain high precision, we used only the most characteristic words in the cluster, focusing on the top 30 keywords, even though using more keywords could have detected other potential relationships. High recall enlarges the possibility of finding a novel combination of research ideas but reduces the efficiency of exploration. Resolving the tradeoff between recall and precision is an issue that should be addressed in future studies to improve the methodology of text analysis.

We must also note that this study is a case study in fuel cells and ammonia synthesis. We demonstrated its effectiveness and validity by

extracting common research fields with shared terms but few shared citations, resulting in a novel research idea. The effectiveness of our approach was validated in a recent publication. However, our analysis was based on studies published in or before 2012; it successfully extracted a novel idea (Nafion and a platinum catalyst supported by carbon (Pt/C)), whose effectiveness has been validated in a recent publication. However, the general effectiveness of our approach should be tested on other cases.

## 5. Conclusion

We proposed a method to help researchers create novel research ideas using bibliometrics. Two clusters, with a high level of keyword similarity, generally use similar techniques and are interactive when it comes to techniques. Hence, there is a strong possibility that techniques used in one area can be passed on to the other area. In the case of fuel cells and ammonia synthesis, clusters with high levels of keyword similarity included “catalyst on carbon” and “ammonia synthesis in ambient conditions.” These clusters use very similar technology, and it is very likely that techniques applied in one area can also be used in the other. The possibilities were investigated through a review of recent publications. Indeed, the recent publications demonstrated that PEFC techniques enhance the performance of electrochemical ammonia synthesis, in which these areas have a high level of keyword similarity. Previous literature on bibliometrics has tended to describe the past and current status of a research field; by contrast, our approach combines explicit citation analysis and implicit text analysis, not only to extract common research topics from distant research fields but also to support the development of novel research ideas.

## Acknowledgments

This research was partially supported by the Science for RE-designing Science, Technology, and Innovation Policy (SciREX) (13413265), the Research Institute of Science and Technology for Society (RISTEX), and the Japan Science and Technology Agency (JST).

## References

- Dalpe, R., Anderson, F., 1995. National priorities in academic research—strategic research and contracts in renewable energy. *Res. Policy* 24, 563–581.
- Ho, J.C., Saw, E.C., Lu, L.Y.Y., Liu, J.S., 2014. Technological barriers and research trends in fuel cell technologies: a citation network analysis. *Technol. Forecast. Soc. Chang.* 82, 66–79.
- Ittipanuvat, V., Fujita, K., Sakata, I., Kajikawa, Y., 2014. Finding linkage between technology and social issue: a literature based discovery approach. *J. Eng. Technol. Manag.* 32, 160–184.
- Kajikawa, Y., Takeda, Y., 2008. Structure of research on biomass and bio-fuels: a citation-based approach. *Technol. Forecast. Soc. Chang.* 75, 1349–1359.
- Kajikawa, Y., Abe, K., Noda, S., 2006. Filling the gap between researchers studying different materials and different methods: a proposal for structured keywords. *J. Inf. Sci.* 32, 511–524.
- Kajikawa, Y., J. Y., Takeda, Y., Matsushima, K., 2008. Tracking emerging technologies in energy research: toward a roadmap for sustainable energy. *Technol. Forecast. Soc. Chang.* 75, 771.
- Katz, J.S., Martin, B.R., 1997. What is research collaboration? *Res. Policy* 26, 1–18.
- Kordali, V., Kyriacou, G., Lambrou, C., 1673–1674. Electrochemical synthesis of ammonia at atmospheric pressure and low temperature in a solid polymer electrolyte cell. *Chem. Commun.* 2000.
- Kostoff, R.N., Tshiteya, R., Pfeil, K.M., Humenik, J.A., 2002. Electrochemical power text mining using bibliometrics and database tomography. *J. Power Sources* 110, 163–176.
- Kostoff, R.N., Tshiteya, R., Pfeil, K.M., Humenik, J.A., Karypis, G., 2005. Power source roadmaps using bibliometrics and database tomography. *Energy* 30, 709–730.
- Lan, R., Irvine, J.T.S., Tao, S.W., 2013. Synthesis of ammonia directly from air and water at ambient temperature and pressure. *Sci. Rep.* 3, 1145.
- Nakamura, H., et al., 2014. Shedding light on a neglected area: a new approach to knowledge creation. *Sustain. Sci.* 9, 193–204.
- Naoki Shibata, Y.K., Sakata, Ichiro, 2010. Extracting the commercialization gap between science and technology; case study of a solar cell. *Technol. Forecast. Soc. Chang.* 77, 1147.
- Naoki Shibata, Y.K., Sakata, Ichiro, 2011. Detecting potential technological fronts by comparing scientific papers and patents. *Foresight* 13, 51–60.
- Newman, M., 2004. Fast algorithm for detecting community structure in networks. *Phys. Rev. E* 69.
- Ogawa, T., Kajikawa, Y., 2015. Assessing the industrial opportunity of academic research with patent relatedness: a case study on polymer electrolyte fuel cells. *Technol. Forecast. Soc. Chang.* 90, 469–475.
- Saadatjou, N., Jafari, A., Sahebdehfar, S., 2015. Ruthenium nanocatalysts for ammonia synthesis: a review. *Chem. Eng. Commun.* 202, 420–448.
- Schumpeter, J., 1934. *The Theory of Economic Development*. Harvard University Press, Cambridge.
- Shibata, N., Kajikawa, Y., Takeda, Y., Matsushima, K., 2009. Comparative study on methods of detecting research fronts using different types of citation. *J. Am. Soc. Inf. Sci. Technol.* 60, 571–580.
- Shibata, N., Kajikawa, A., Sakata, I., 2011. Measuring relatedness between communities in a citation network. *J. Am. Soc. Inf. Sci. Technol.* 62, 1360–1369.
- Small, H., 2006. Tracking and predicting growth areas in science. *Scientometrics* 68, 595–610.
- Swanson, D.R., 1986. Fish oil, Raynauds syndrome, and undiscovered public knowledge. *Perspect. Biol. Med.* 30, 7–18.
- Tijssen, R.J.W., 1992. A quantitative assessment of interdisciplinary structures in science and technology—co-classification analysis of energy research. *Res. Policy* 21, 27–44.
- Xu, G.C., Liu, R.Q., 2009.  $\text{Sm}_{1.5}\text{Sr}_{0.5}\text{MO}_4$  (M=Ni, Co, Fe) cathode catalysts for ammonia synthesis at atmospheric pressure and low temperature. *Chin. J. Chem.* 27, 677–680.
- Zheng, Y., Jiao, Y., Jaroniec, M., Jin, Y., Qiao, S.Z., 2012. Nanostructured metal-free electrochemical catalysts for highly efficient oxygen reduction. *Small* 8, 3550–3566.

**Dr. Takaya Ogawa** holds a postdoctoral fellowship from the Japan Society for the Promotion of Science (JSPS) and works at the Department of Chemistry, Massachusetts Institute of Technology, and the Material Research Center for Element Strategy, Tokyo Institute of Technology. He holds bachelor's and master's degrees in engineering from the University of Tokyo, a master's degree in management of technology, and a PhD in science from the Tokyo Institute of Technology. He has multidisciplinary expertise in quantum chemistry, materials science and processing, technology management, and information processing. His current research interests include energy-related technologies, R & D management, and information processing.

**Dr. Yuya Kajikawa** is an associate professor at the Graduate School of Innovation Management, Tokyo Institute of Technology. He is also a visiting professor at the Nagoya University Strategic Innovation Office. He received his bachelor's degree, master's degree, and PhD from the University of Tokyo. His research interests include the development of methodology for technology and innovation management. He has contributed several papers to peer-reviewed journals and conference proceedings, covering a variety of disciplines such as engineering, information science, environmental science, and technology and innovation management. He is an associate editor of the journal *Technological Forecasting and Social Change*.