

## Global Trends in Molecular Diffusion Research from 2001 to 2017: A Bibliometric Analysis

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### Abstract

Molecular diffusion is one of the most important topics in transport phenomena because it refers to the transport of material in a stagnant fluid or across streamlines of a fluid, which is the fundamental basis of mass transfer. This phenomenon is involved in all the unit operations of chemical engineering. It is necessary for the development of new valuable researches in the mentioned topic so, it is essential to assess its tendency toward research. In this study, it was completed an analysis of the research development of Molecular diffusion from 2001 to 2017, using the software HistCiteTM. This study evaluated a total of 2055 publications related to Molecular diffusion which were used to track the trends of publications outputs, countries, main language, authors, institutions, main journal, and keywords. The USA, the Republic of China, and Japan were the top 3 most productive countries with 563, 232, and 215 publications respectively. The most productive institution was the Russian Academy of Sciences followed by Hokkaido University in Japan and the Chinese Academy of Sciences. The journals with the most significant number of articles were the Journal of Chemical Physics, the Journal of Physical Chemistry B, and the Abstracts of Papers of the American Chemical Society.

**Keywords:** Bibliometrics, molecular diffusion, research trend

## **1. Introduction**

The phenomenon of mass transfer is a highly relevant subject in the industry because it is involved in all the unit operations. Besides, it is present in most industrial processes like such as absorption, distillation, drying, leaching, and membrane filtration. To have a complete understanding of mass transfer, it is necessary to have a solid knowledge of molecular diffusion because it is the fundamental transport mechanism. The more the knowledge about molecular diffusion, the higher the efficiency in the operation of industrial processes. There is a large number of researches about molecular diffusion. It was studied the effects of temperature and solid concentration on the transport properties of the solid-gas system SiO<sub>2</sub>/H<sub>2</sub>O [1]. A desorption process applying direct molecular diffusion and micro-mixing from a solution flow confined within microchannels with smooth walls was experimentally studied [2]. Molecular diffusion has been implemented during food processing [3, 4]. It has a broad application in the care of the environment like wastewater treatment [5], and dust treatment [6]. It makes necessary to continue researching this topic. It is essential to perceive the direction that is taking the study in molecular diffusion to give the best route that researchers must follow to provide the highest scientific contribution possible. It is made by examining a significant amount of information with the tool named bibliometric that helps to detect the scientific production and research inclinations of different fields or topics. With this process, all the information is measured, organized, evaluated, studied, and compared with the aid of additional computational tools. In this study, it is presented the trend of research of molecular diffusion by screening this theme of investigation worldwide from scientific documents published from 2001 to 2017. It was completed using a bibliometric analysis with the help of specialized software. The purpose was to measure, assess and compare the participation of recognized institutions, scientific journals, researchers, and countries around the world and in relation to their interest in molecular diffusion to follow the direction of research in this subject.

## **2. Methodology**

This study was made collecting the information on a large number of scientific documents. This information was given by the online based scientific citation indexing database Web of Science. To obtain the data, it was used a computational tool that makes the connection of all the bibliographic information (titles, dates, author names, author addresses, references, etc.) to perform bibliometric analysis and visualization tasks. It was found a total of 2055 documents about research in molecular diffusion. The criteria of evaluation used for the acquired publications in the database were the next: year of publication, main journals, most productive institutions, most productive countries, author keywords, and most productive authors. It was implemented a software of data analysis to adapt the results according to the settings of the user. To have a better comprehension of the results, they were grouped into tables and graphs of different types to have a better insight into the trend.

### 3. Results and Analysis

#### 3.1. Publication outputs

The range of time from 2001 to 2017 was taken to make a bibliometric analysis on molecular diffusion, where a total of 2055 documents were identified. The type of document most commonly used was the article type with a total of 1726 publications (84.0%), followed by proceedings papers with 157 publications (7.64%), meetings abstract with 112 publications (5.44%), reviews with 26 publications (1.23%), corrections with 10 publications (0.49%), letter with 8 publications (0.39%), and editorial material with 4 publications (0.19%). The predominant language was English with 1997 publications out of 1279, representing the 97.19%, followed by Chinese (37), French (6), Korean (4), and Portuguese, Russian, and Spanish with 2. Figure 1 shows an increase in the number of publications from 2001 to 2017 presenting a linear behavior with a slope of 5.27 publications per year. This topic had a raise in research publication of 143% from 2001 to 2017.

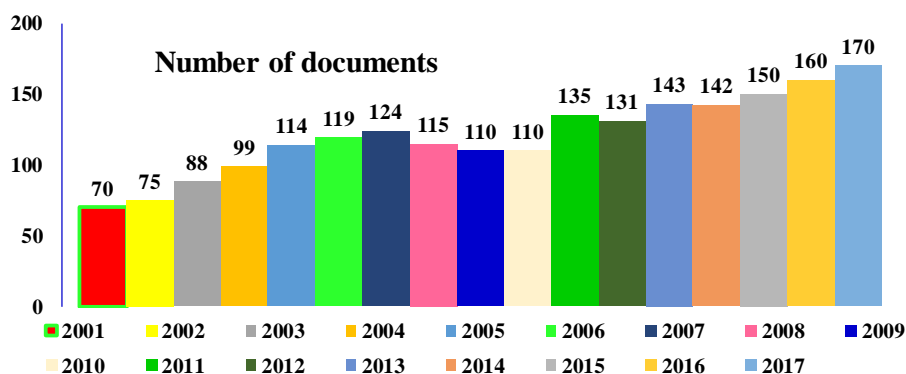


Figure.1 Number of published documents from 2007 to 2017.

Table 1 presents the ten major scientific journals with the highest production of papers in the mentioned topic. NP denotes the number of publications, TLCS refers to the total local citation score, TGCS is the total global citation score. The Journal of Chemical Physics was the first with 176 publications that is the 8.6% of the total number of documents. Journal of Physical Chemistry B follows it with 109 documents (5.3%), and Abstracts of Papers of the American Chemical Society with 55 documents (2.7%). 7 of the top 10 journals with the highest production have the highest TLCS values. When assessing with the quality parameter TLCS/NP, the best journal is Journal of Physical Chemistry B.

Figure 2b shows the countries that produced the highest number of publications from 2007 to 2017, where the USA registered 563 representing the 27.41% of the total NP. It is followed by the Republic of China with 232 documents (11.30%), Japan with 215 (10.46%), and Germany with 163 (7.95%). It can be seen that these countries are highly industrialized and have many important centers of research

which are evidenced in a large number of studies.

Table 1. Top ten journals with the highest quantity of publications

#	Journal	NP	NP %	TLCS	TGCS	TLCS/NP
1	Journal of chemical physics	176	8.6%	124	1897	0.70
2	Journal of physical chemistry B	109	5.3%	382	1954	3.50
3	Abstracts of papers of the American Chemical Society	55	2.7%	92	1534	1.67
4	Biophysical journal	47	2.3%	64	1262	1.36
5	Physical review B	45	2.2%	17	534	0.38
6	Journal of physical chemistry C	40	1.9%	12	462	0.30
7	Polymer	40	1.9%	109	456	2.73
8	Chemical physics letters	34	1.7%	32	337	0.94
9	Langmuir	34	1.7%	45	493	1.32
10	Physical chemistry chemical physics	30	1.5%	96	369	3.20

The countries presented in figure 2 refers to developed and developing countries. Their advanced technology and capacity of research help them to make many studies on different topics promoting the successful management of knowledge, and ideas, especially on molecular diffusion. Countries of figure 2b have lots of industries in the food, chemical, and environmental sectors where this topic is highly applied. As can be seen figure 2a and b, The USA has the highest values. It indicates that they have both, high productivity and high quality of research, which is coherent with the high technology of its research institutions.

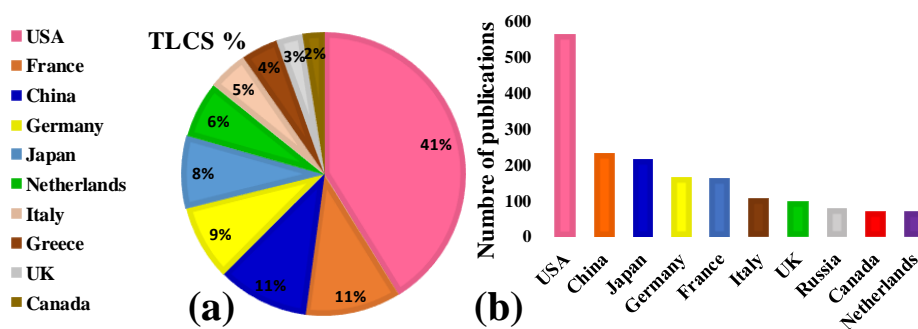


Figure 2 Top 10 countries with the a) highest proportion of TLCS b) highest number of published documents

Table 2 shows the institutions with the highest number of publications about molecular diffusion. The top two institutions are the Russian Academy of Sciences with 43 publications and Hokkaido University in Japan with 34 papers.

Table 2. Top ten most productive institutions from 2007 to 2017

#	Institution	NP	NP %	TLCS	TGCS	TLCS/NP
2	Russian Acad Sci	43	2.09%	5	397	0.11
3	Hokkaido Univ	34	1.67%	42	365	1.21
4	Chinese Acad Sci	32	1.57%	28	140	0.86
5	Univ Leipzig	32	1.57%	28	345	0.86
6	Tokyo Inst Technol	28	1.36%	9	227	0.33
7	Univ Amsterdam	28	1.36%	111	768	3.97
8	Kyushu Univ	26	1.26%	18	76	0.72
9	Univ Texas	24	1.15%	18	219	0.78
10	Univ Bordeaux 1	22	1.05%	65	170	3.01
11	Univ Calif Berkeley	22	1.05%	65	315	3.01

The Russian Academy of Sciences has the Institute of Macromolecular Compounds, The Institute of High Temperature Electrochemistry, and the Semenov Institute of Chemical Physics where investigations about molecular diffusion are done. On the other hand, Hokkaido Univ has Institute of Low Temperature Science and the division of Chemical Process Engineering which aims at researching in the important technical areas of industrial organic chemistry and chemical engineering from molecular through process design. On the other hand, the Chinese Academy of Science makes research of molecular diffusion in the Wuhan Institute of Physics and Mathematics, and in the State Key Laboratory of Polymer Physics and Chemistry.

Three of the top ten institutions with the highest quantity of published papers appear in the list of the top ten institutions with the highest TLCS values evidencing the high quality of their research in molecular diffusion. These universities are The University of Amsterdam in the Netherlands, The University of Bordeaux 1 in France, and University of California, Berkeley.

Table 3 Top twenty authors keyword from 2007 to 2017

#	Keyword	NP	TLCS	#	Keyword	NP	TLCS
1	Molecular	954	369	11	Using	49	62
2	Diffusion	953	369	12	Carbon	48	34
3	Dynamics	420	237	13	Nmr	46	16
4	Simulation	173	111	14	Weight	44	8
5	Simulations	130	101	15	Structure	40	9
6	Self	90	48	16	Based	38	4
7	Water	68	15	17	Effect	38	6
8	Coefficients	56	30	18	Model	38	11
9	Surface	54	9	19	Polymer	37	14
10	Liquid	49	15	20	Mixtures	35	42

The examination of author keywords gives details about article topics and the tendency areas of particular research interest. Table 3 shows the top keywords appearing in articles from 2007 to 2017 with a total of 2175 keywords where the most important are molecular, diffusion, dynamics, and water. As can be seen, water is the primary fluid where research on this topic is made. However, simulations in this subject are of high importance to predict the behavior of molecular diffusion in different processes.

### 3.2. Most productive authors

The authors with the highest number of publications were Jörg Kärger from the Institute for Experimental Physics I, Faculty of Physics and Earth Science, University of Leipzig in Germany, with 31% of the total publications of the ten top authors, followed by Rajamani Krishna from Van 't Hoff Institute for Molecular Sciences in the University of Amsterdam with 22%, see figure 3a.

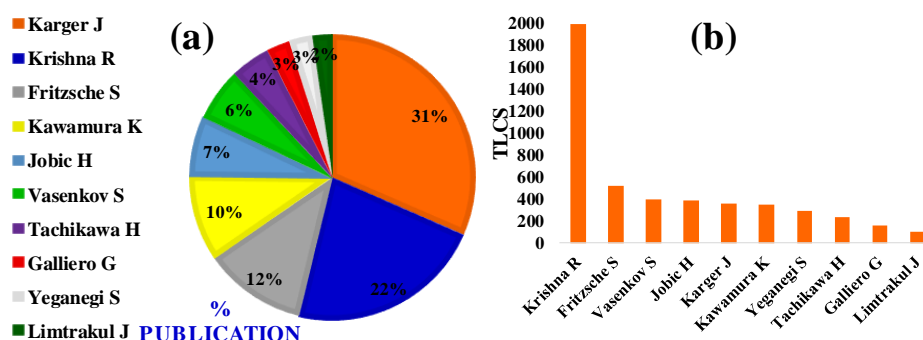


Figure 3. Top 10 authors with the a) highest number of papers b) highest proportion of TLCS

Besides having the highest number of publications, Kärger and Krishna are in the list of the top 10 authors with the highest TLCS values, 357 and 1995 respectively, see figure 3b. It guarantees the high quality of their papers.

## 4. Conclusions

A bibliometric analysis of number of publications, major journals, international productivity, most productive authors and keyword using a specialized software was used to follow the worldwide trend in the research productivity associated to molecular diffusion from 2001 to 2017 and provide the best direction that researchers must follow to give the highest scientific contribution possible. The number of publications had an increase with a slope of 5.27 documents per year. This research subject had a rise in research publication of 143% from 2001 to 2017. The USA, Republic of China, Japan, and Germany were the countries leaders in production of scientific documents with 563, 232, 215 and 163 publications

respectively. These countries with the highest TLCS values were The USA with 712, and France with 190. The top 2 institutions with the highest article production were the Russian Academy of Sciences with 43 publications and Hokkaido University in Japan with 34 documents. The journals with the maximum number of articles were the Journal of Chemical Physics with 176 publications corresponding to the 8.6% of the total number of documents, followed by the Journal of Physical Chemistry B with 109 documents (5.3%). The author with the highest quantity of publications was Jörg Kärger from the University of Leipzig in Germany, with 31% of the total publications of the ten top authors

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