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Top Cited Articles in Thermodynamic Research

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Abstract—The 5,320 top cited articles published between 1902 and 2010 in thermodynamic field were identified and characterized using Science Citation Index Expanded. The analyzed aspects covered characteristics of languages, publication years, Web of Science categories, journals, countries/territories, institutions, and authors. These articles were cited a mean number of 210, ranging from 110 to 399 times, with most of the articles in the 1990s and 2000s. *Journal of the American Chemical Society* was the most productive journal, followed by *Journal of Chemical Physics*, and *Physical Review Letters* in 686 journals. Three topmost categories of the 130 Web of Science categories were multidisciplinary chemistry, biochemistry and molecular biology, and physical chemistry. The top cited articles originated from 1,936 institutions of 63 countries. Eight industrial countries: the USA, the UK, Germany, France, Canada, Japan, Italy, and Russia, took the lead with an overwhelming majority (87%), especially about three fifths for the USA. University of California, Harvard University, and Massachusetts Institution of Technology all from the USA led all the institutions. K.S. Pitzer, P.J. Flory (Nobel laureate), and P.A. Kollman advanced the development of thermodynamic field. Moreover, the most influential articles in the history and in the latest year with their citation life cycles were examined to provide some hints for research focuses and trends. Wigner function has been attractive and will probably continue to be popular in the thermodynamic field. Some emerging concerning related to frequency scale factors, OPLS all-atom force field, entanglement between two or more quantum objects, and some softwares including VAMP, NMRPipe, GRASP2, AutoDock, DMol^3, and Maxent are likely to receive more attention in the near future.

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1. INTRODUCTION

As early as the 18th century, the thermodynamics investigation has been conducted in terms of heats of chemical reaction [1]. The early studies in the beginning of the 19th century paid attention to atmosphere [2], electro-chemical processes [3], bioelectric currents [4], heat engines [5], and mechanism basis [6]. Thermodynamics advanced dramatically in the 1960s and 1970s, primarily in the area of critical phenomena [7]. In recent years, thermodynamic research has been studied of diverse interests, such as glass-forming substances [8], DNA structural motifs [9], nanoclusters [10], a universal Fermi gas [11], and meat proteins [12]. Many studies have contributed to the long-term development of the thermodynamic field [13–15]. It is interesting to get a full picture of the field of thermodynamics with such a long history and diverse studies.

Recently, top cited articles have been employed to reveal the recognition of scientific advancement and to give a historic perspective on the scientific progress [16, 17]. Top cited articles were considered as "classic citations" [18]. Various studies have attempted to identify and analyze the "citation classics," especially in medical fields, such as leading dermatologic journals [19], the *Journal of Molecular Biology* [20], anaesthesia and pain journals [21], and ophthalmology journals [17]. Top cited articles in the field of thermodynamics were retrieved for investigation of this study.

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Top cited articles have been usually evaluated of the following aspects: publication year [22, 23], journals [17, 24], countries and institutions [16, 23], and authors [22, 24]. Particularly, five indicators including number of total publications, independent publications, collaborative publications, first author publications, and corresponding author publications have been developed to characterize countries and institutions in a series studies, related to research topics, for example, risk assessment [25] and global climate change [26], as well as comparison of universities [27], and publication characteristics of country [28]. Furthermore, research focuses were also investigated as an important concerning for the top cited papers [29, 30]. TC"year," such as TC2009, the cited times of one article received from its published year to 2009, was recently introduced to evaluate the impact of articles since it is invariable and comparable [27, 31]. Interestingly, citation life cycles of top cited articles were attached importance to obtain more detail of the impact characters [32, 33].

The articles analyzed top cited articles with at least 100 citations from the field of thermodynamics over the last 110 years. This study not only identified the characteristics of languages, publication years, Web of Science categories, journals, countries/territories, institutions, and authors, but also revealed research focuses and trends by top articles in the long history and in latest year.

2. METHODOLOGY

2.1. Data Collection

Documents used in this study were derived from the Science Citation Index Expanded (SCI-Expanded) database of the Web of Science (WoS), the Thomson Reuters. Keywords "thermodynamic," "thermodynamics," "free energy," "enthalpy," and "entropy" were searched in terms of topic (including four parts: paper title, abstract, author keywords, and KeyWords Plus) based on SCI-Expanded (updated 16 March 2012). The data collection process is illustrated in Fig. 1. Total 323,578 documents were downloaded by this filter. Article (272,672) was the only document type for further analysis. Another two recently developed filters: *TC2011* and the front page were employed to retrieve articles. *TC2011* $\geq$ 100 selected the articles as the top cited articles. The total number of times article cited from its publication to 2011 was recorded as *TC2011* [27, 31]. Another filter, the front page, meant only the articles with the searching keywords in their front page including article title, abstract, and author keywords were searched out. KeyWords Plus provides search terms extracted from the titles of papers cited in each new article listed in *Current Contents* [34], therefore, the articles, which can only be searched out by KeyWords Plus, were more likely unrelated to thermodynamic. The articles with searching keywords only appeared in KeyWords Plus were excluded. Finally, 5,320 (1.6%) articles were considered to be the top cited articles. The 5,320 articles having search keywords in the front page and having *TC2011* $\geq$ 100 were retrieved for further analysis. The records were downloaded into spreadsheet software, and additional coding was manually performed using Excel in subsequent analysis.

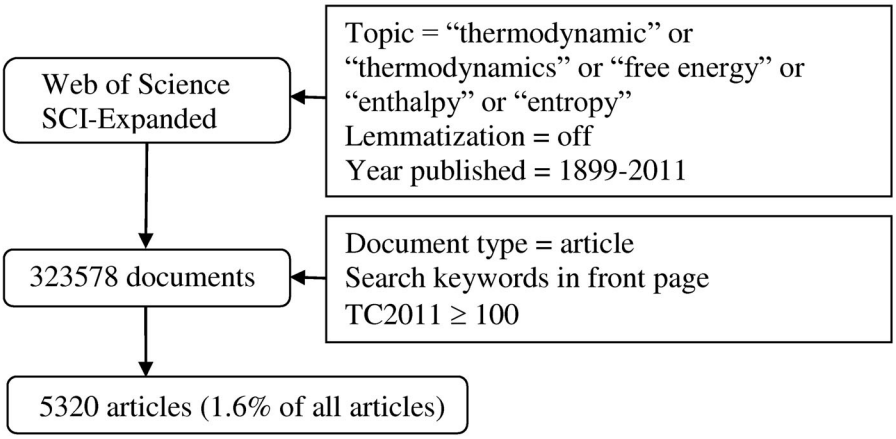

Fig. 1. Schematic for searching thermodynamic research in Science Citation Index Expanded.

2.2. Pretreatment and Indicators

The items of country downloaded from WoS need to be categorized based on the facts before analysis. Articles originating from England, Scotland, Northern Ireland, and Wales were reclassified as being from the United Kingdom (UK). Federal Republic of Germany (Fed Rep Ger), German Democratic Republic (Ger Dem Rep), West Germany, and Germany were reclassified as being from Germany. USSR and Russia were reclassified as being from Russia. Czechoslovakia and Czech Republic were also reclassified as being from Czech Republic. Yugoslavia and Croatia were also reclassified as being from Croatia. Articles from Hong Kong published before 1997 were included in the China category. The contributions from institutions and countries/territories were identified by the appearance of at least one author in the publications. Collaboration type was determined by the addresses of the authors. The articles were classified by four types for country/territory and institution. (1) The term "single country article" was assigned if the researchers' addresses were from the same country. The term "single institution article" was assigned if the researchers' addresses were from the same institution. (2) The term "internationally collaborative article" was designated to those articles that were coauthored by researchers from multiple countries [35]. The term "inter-institutionally collaborative article" was assigned if authors were from different institutions. (3) The term "first author article" was assigned if the first author was from the country/territory or institution for analysis; or if one person was assigned as the first author for the author for analysis. (4) The term "corresponding author article" was assigned if the corresponding author was from the country/territory or institution for analysis; or if one person was assigned as the corresponding author for the author for analysis. *TP*, *SP*, *CP*, *FP*, and *RP* are the number of total articles, "single country articles" or "single institution articles," "internationally collaborative articles" or "inter-institutionally collaborative articles," "first author articles" and "corresponding author articles" for a country/territory, institution or an author, respectively.

3. RESULTS AND DISCUSSION

3.1. Characteristics

3.1.1. Languages and Publication Outputs

The total 5,320 articles were published in four languages. As expected, English (5,302 articles; 99.6%) was the main language. The other three languages were German (16), French (1), and Russian (1). The percentage of English was greater than the total population of publications in some studies, such as 93% in acupuncture research [36] and 94% in desalination research [37].

These top cited articles ($TC2011 \geq 100$) were published in a long period of 109 years from 1902 to 2010. Figure 2 illustrates publication outputs and citations per publication (*CPP*) by decades. The publication outputs of decades increased during the 1900s–1980s, and soared to a peak of 2,555 articles in the 1990s, but then dropped in last two decades. The two most productive decades were 1990s (2,555; 48%), and the 2000s (1,313; 25%), while the three least productive decades were the 1900s, 1910s, and 2010s, with a total number of eight articles. The mean number of *CPP* was 210, ranging from 399 to 110. Except the 1900s, the *CPPs* of other 11 decades showed an increasing trend during 1910s–1940s, but decreased during the 1950s–2010s. The high *CPPs* in the 1900s may be explained in part by the small size of scientific production and their high citations. The 1910s with 36 article and the 1930s with 68 articles had the higher *CPPs* of 394 and 399, which can be attributed to the articles by Wigner with a $TC2011 = 4{,}758$ in 1932 and three top articles with *TC2011* more than 2000 in the 1930s.

The top articles with $TC2011 > 2000$ were identified in Fig. 3 according to their published years. Total 22 articles included one each in the 1930s, 1950s, and 1980s, two in the 1970s, three in the 1940s and 1960s, and 11 in the 1990s. The decade of the 1990s took a half of articles. No top article was found in the earliest decades of the 1900s, 1910s. There were also no top articles in the latest two decades of the 2000s and 2010s. This performance may possibly due to the evidence that it needs time to accumulate citations [20]. The performance of 22 articles with $TC2011 > 2010$ was consistent with the above performance of total 5,320 articles, and also can explain it to some extent.

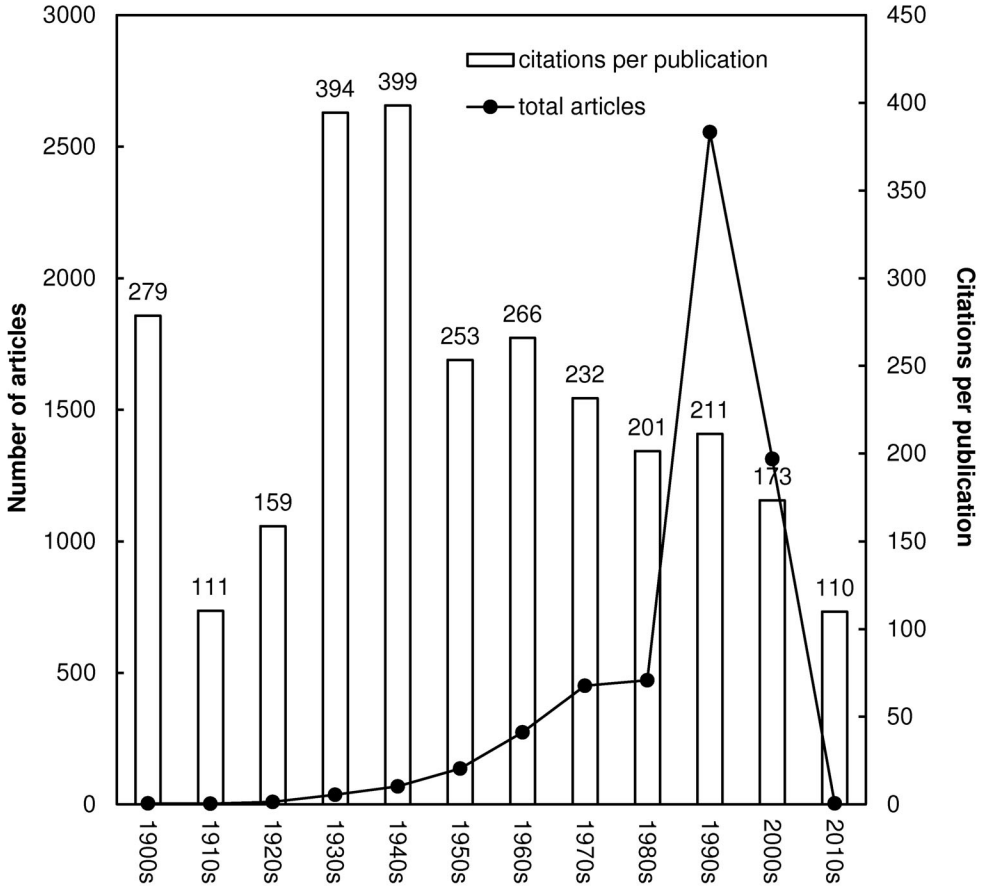

Fig. 2. Number of articles and citation per articles by decades.

3.1.2. Web of Science Categories and Journals

According to Journal Citation Reports (JCR) Science Edition, it indexes 8,073 journals with citation references across 174 scientific categories in 2010. Total 120 categories were found. Categories were sorted by the number of articles into three zones, each with about one-third of all articles, the number of categories in each zone was found to be proportional to $1 : n : n^4$. The categories of zone 1 could obviously be recognized as the core categories. In this study, the categories in descending order in terms of their published articles were sorted, and the categories were divided into three "zones." Zone 1, representing the most productive third of the total articles, contained 4 categories or 3.3% of 120 categories. Zone 2, representing the next most productive third of total articles, contained 9 categories or 7.5% of 120 categories. Zone 3, representing the least productive third of total articles, contained 107 categories or 89% of 120 categories. The four core categories were multidisciplinary chemistry with 690 articles (13%), biochemistry and molecular biology with 676 articles (13%), physical chemistry with 636 articles (12%), and multidisciplinary sciences (467; 8.8%). By considering 120 categories into different disciplines, the equal categories of 13 fell into chemistry and physics, taking nearly the same high percentages of 42% and 41% of total articles, respectively. More categories and assigned top cited articles were related to science with 23 categories (18% articles) than engineering with 13 categories (6.4% articles).

The top cited articles were published by 686 journals. Of these 686 sources, 331 (48%) journals contained only one article, 286 (42%) journals contained 2–10 articles, 58 (8.5%) journals contained 11–100 articles, 12 (1.7%) journals contained more than 100 articles. The top 20 journals took account of more than half (53%) the articles. Characteristics of top 20 journals with the most top cited articles

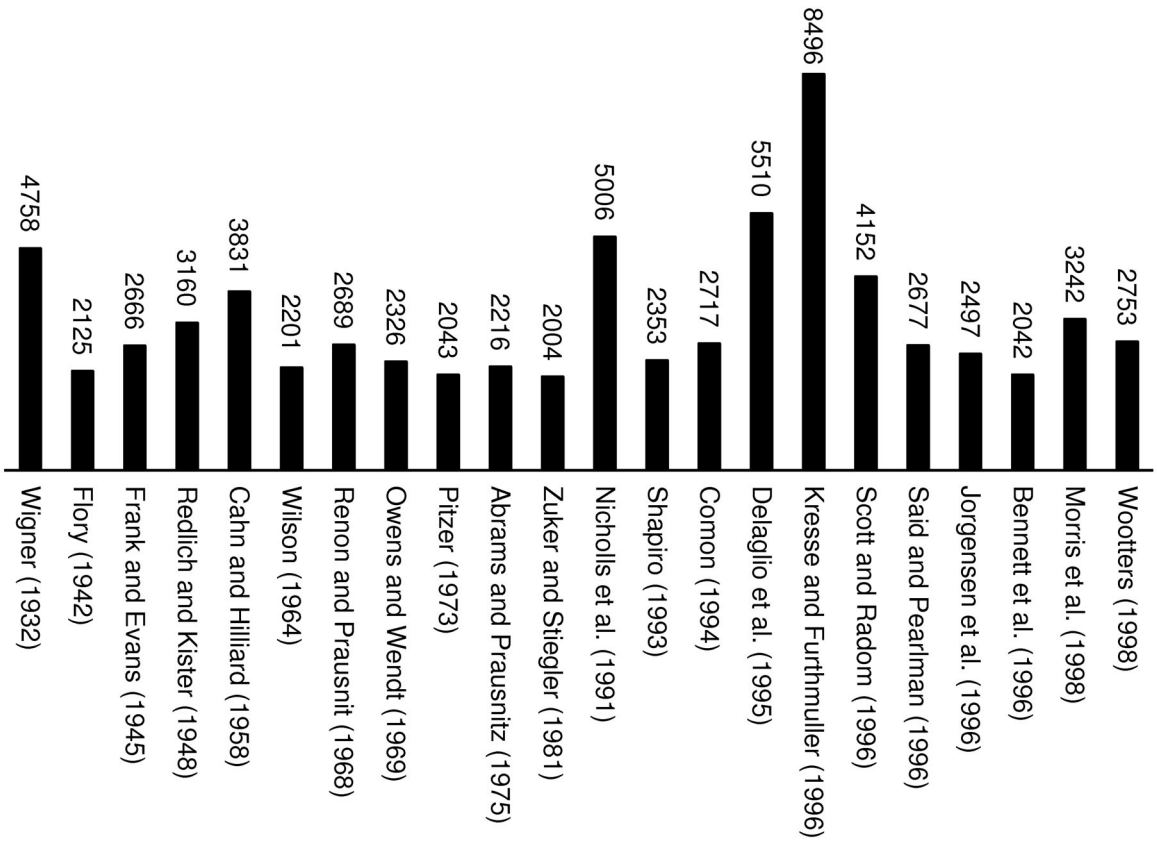

Fig. 3. Top cited articles with *TC2011* > 2000 according to the order of their publication years.

are displayed in Table 1. The journals' impact factors were also exhibited to characterize them since reputation of a journal attached much attention for the authors and editors [38]. The impact factor (IF) of a journal was determined for each document as reported in the Journal Citation Reports 2010. Of note: the impact factor from the 6th position *Journal of Physical Chemistry* was not available using JCR 2010, because *Journal of Physical Chemistry* has split into *Journal of Physical Chemistry A*, *Journal of Physical Chemistry B*, and *Journal of Physical Chemistry C*. *Physical Chemistry Chemical Physics* (1999 to present) included its formers: *Transactions of the Faraday Society* (1905–1971), *Journal of the Chemical Society, Faraday Transactions I* (1972–1989), *Journal of the Chemical Society, Faraday Transactions II*, and *Journal of the Chemical Society, Faraday Transactions* (1990–1998). *Acta Crystallographica*, established in 1948, was separated into Section A and Section B in 1967.

Journal of the American Chemical Society (419) was the most productive journal, followed by *Journal of Chemical Physics* (290), *Physical Review Letters* (258), *Biochemistry* (214), and *Proceedings of the National Academy of Sciences of the United States of America* (210) with more than 200 articles. All of the 20 journals ranked upper middle in its Web of Science category using IF. Particularly, seven journals including *Journal of the American Chemical Society*, *Physical Review Letters*, *Proceedings of the National Academy of Sciences of the United States of America*, *Nature*, *Macromolecules*, *Science*, and *Geochimica et Cosmochimica Acta* ranked top 10% in its categories. As expected, top cited articles were published in thermodynamic journals with high impact factors, similar to the phenomenon in the study related to anesthetic [16]. Top cited papers are mainly presented in high impact journals [33]. The leading journals attracted the top cited publications, which in turn maintained the high impact factor for these journals [39]. However, some top cited articles were published in some journals with low impact factors. For example, some articles with TC2011 > 1,000 could also be found in journals with lower impact factors, such as *Journal of Elasticity* (IF = 1.160), *Clays and Clay Minerals* (IF = 1.631), *Communications in Mathematical Physics* (IF = 2.000), and *Surface Science* (IF = 2.011). Moreover, the three highest impact factors were found in *Acta*

Table 1. Characteristics of top 20 journals with the most top cited articles

Journal	TP[a]	%	IF2010	Web of Science category (Position by impact factor/total journals)
Journal of the American Chemical Society	419	7.9	9.019	Multidisciplinary chemistry (11/147)
Journal of Chemical Physics	290	5.5	2.921	Atomic, molecular, and chemical physics (7/33)
Physical Review Letters	258	4.8	7.621	Multidisciplinary physics (5/80)
Biochemistry	214	4.0	3.226	Biochemistry and molecular biology (120/286)
Proceedings of the National Academy of Sciences of the United States of America	210	3.9	9.771	Multidisciplinary sciences (3/59)
Journal of Physical Chemistry	169	3.2	N/A[b]	N/A[b]
Physical Review B	146	2.7	3.774	Condensed matter physics (13/68)
Nature	134	2.5	36.104	Multidisciplinary sciences (1/59)
Macromolecules	131	2.5	4.838	Polymer science (5/79)
Journal of Molecular Biology	124	2.3	4.008	Biochemistry and molecular biology (86/286)
Physical Review D	106	2.0	4.964	Astronomy and astrophysics (8/55); particles and fields physics (5/27)
Science	94	1.8	31.777	Multidisciplinary sciences (2/59)
Journal of Physical Chemistry B	74	1.4	3.603	Physical chemistry (32/127)
Astrophysical Journal	74	1.4	6.063	Astronomy and astrophysics (6/55)
Physical Chemistry Chemical Physics	74	1.4	3.454	Physical chemistry (34/127); atomic, molecular, and chemical physics (5/33)
Biophysical Journal	73	1.4	4.218	Biophysics (18/73)
Physical Review A	59	1.1	2.861	Optics (9/78); atomic, molecular, and chemical physics (8/33)
Geochimica et Cosmochimica Acta	54	1.0	4.101	Geochemistry and geophysics(4/77)
Physical Review E	52	1.0	2.352	Fluids and plasmas physics (8/31); mathematical physics (4/54)
Langmuir	48	0.90	4.268	Multidisciplinary chemistry (24/147); physical chemistry (29/127); multidisciplinary materials science (26/225)

[a]Total number of top cited articles. [b]Not available.

Crystallographica Section A (IF = 54.333) with five top cited articles, *Reviews of Modern Physics* with seven articles (IF = 51.695), and *Nature Genetics* with two articles (IF = 36.377). The other high impact factor journals such as *Nature* (IF = 36.104) and *Science* (IF = 31.364) also had highly production of top cited articles.

3.1.3. Countries/Territories' Publication Performances

Excluding 598 articles without any author address information on the Web of Science, the 4,722 articles originated from 63 countries. The geographical global distribution of thermodynamic research is

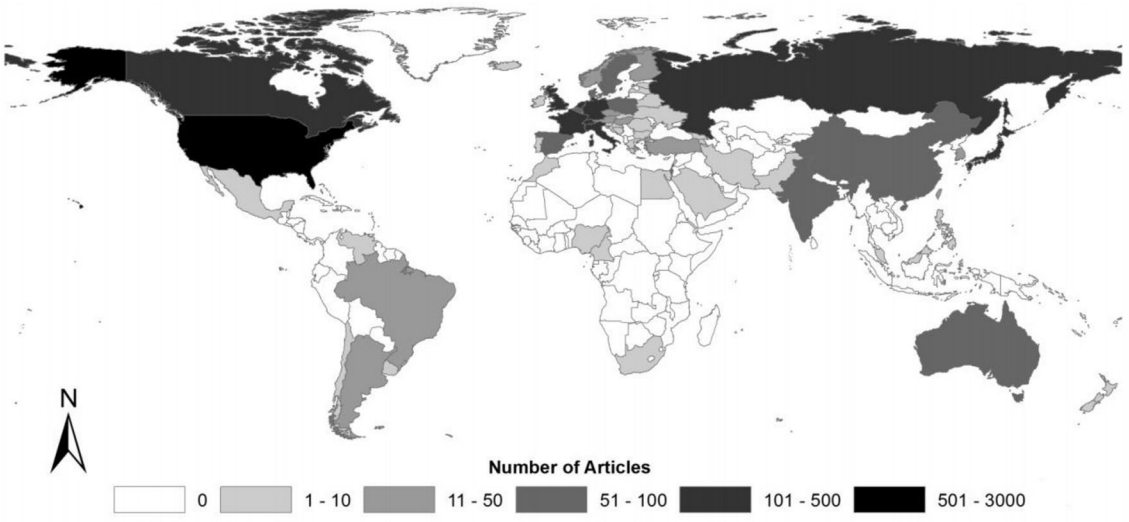

Fig. 4. Global geographical distribution of thermodynamics research outputs.

Table 2. Characteristics of the top 10 productive countries using *TP*, *SP*, *CP*, *FP*, and *RP*

Country	TP	*TP* R (%)	*SP* R (%)	*CP* R (%)	*FP* R (%)	*RP* R (%)	C%
USA	2,880	1 (61)	1 (60)	1 (65)	1 (55)	1 (52)	24
UK	419	2 (8.9)	2 (5.8)	2 (20)	2 (6.3)	2 (6.8)	49
Germany	418	3 (8.9)	3 (5.8)	2 (20)	2 (6.3)	3 (6.7)	49
France	309	4 (6.5)	5 (3.9)	4 (16)	5 (4.1)	4 (4.6)	54
Canada	278	5 (5.9)	4 (4.0)	5 (12)	4 (4.4)	5 (4.0)	46
Japan	205	6 (4.3)	6 (3.6)	9 (7.0)	6 (3.4)	6 (3.8)	36
Switzerland	164	7 (3.5)	7 (2.1)	7 (8.4)	7 (2.5)	7 (2.5)	53
Netherlands	142	8 (3.0)	8 (1.9)	9 (7.0)	8 (2.2)	8 (2.3)	51
Italy	140	9 (3.0)	10 (1.4)	6 (8.6)	9 (2.0)	9 (2.2)	64
Russia	108	10 (2.3)	16 (0.87)	8 (7.3)	13 (1.1)	15 (1.0)	70

shown in Fig. 4. According to their production, the 63 countries were divided into five parts. Particularly, 34 countries (54%) belonged to the first part of 1–10 articles; ten countries (16%) belonged to the second part of 11–50 articles; nine countries (14%) belonged to the third part of 51–100 articles; nine countries (the UK, Germany, France, Canada, Japan, Switzerland, Netherlands, Italy, and Russia) with 14% of all top cited articles belonged to the fourth part of 101–500 articles; and only one country (USA) which published 2,880 articles, belonged to the fifth part of 501–3,000 articles. Although there were only 10 countries, which published more than 100 articles, these 10 countries produced 91% articles. Table 2 shows the characteristics of the top 10 productive countries of five indicators: *TP*, *SP*, *CP*, *FP*, and *RP*. The first author who related to *FP* was the experimenter or author who contributed the most to the study [40, 41]. Corresponding author who related to *RP* made the second largest contribution [42, 43]. The first author contributed the most to the work performed, while corresponding author was the one who contributed the most to the initial conception and supervision [44]. The distribution of country ranks was rather similar. Only slight variation in country rankings by the five indicators was displayed. Some countries' ranks never changed according to these five indicators, such as the USA (1st), UK (2nd), and Switzerland (7th).

The USA dominated, followed distantly by other countries. The USA ranked 1st in independent articles and collaborative articles as well as first author and corresponding author articles, taking about 61% of the total top cited articles. The percentage was much higher than many studies based on all publications with not only top cited articles, such as 18% of desalination research [37], 20% in solid waste [45], 36% of water resources journals [46], and 39% of global climate change [26]. It seems that the USA performed better in the high quality publication. It might be explained partly by the large size of the American scientific publications [47]. There is some evidence that authors and reviewers tend to quote and evaluate USA publications more favorably [48, 49]. The eight major industrialized countries (G8: Canada, France, Germany, Italy, Japan, Russia, the UK, and USA), ranked in the top 10, accounting for 87% over the investigation period. It is not surprising industrialized countries dominated in the top cited articles of thermodynamics. Similarly, the domination of seven major industrialized countries G7 (G8 excluding Russia) have been found in many researches [50, 51]. Moreover, Germany, France, and Russia, which use the languages including German, French, and Russian except English as their mother tongues, were all just listed as top countries. This performance is consistent with the above analysis of languages.

International collaboration played an important role to enhance the impact of articles [52, 53]. With respect to international collaboration, 3,685 (78%) were independent publications, and 1,037 (22%) were internationally collaborative publications. The collaboration rate of top cited articles was greater than that in the total population of publications, including 14% in biosorption technology [54] and acupuncture research [36], 16% in solid waste [45] and desalination research [37], and 18% in financial crisis research [55]. Top cited papers typically involve more collaborative research than what is the normal or average [33]. However, the USA, which dominated in all indicators, had the lowest collaboration rate of 24% of the list. The 10th position Russia had the highest collaboration rate of 70%. Here, the phenomenon is another line of evidence that the magnitude of international co-authorship is weakly dependent on the scientific size of a country [56].

3.1.4. Institutions' Publication Performances

The 4,722 articles were contributed by 1,936 institutions. Of these articles, 2,711 articles (67%) came from independent institution, 2,011 articles (43%) from inter-institutional collaboration, and 1,037 articles (22%) from national collaboration. The inter-institutional collaboration rate differed widely in different disciplines, such as 16% of water resources journals [46], 37% of desalination research [37], 44% in solid waste [45], and 62% of global climate change [26]. In terms of publication outputs of institutions, 1,767 (91%) institutions published 1–10 articles, 137 (7.1%) institutions published 11–50 articles, 16 (0.83%) institutions published 51–100 articles, and 5 (0.26%) institutions published more than 101 articles. Total 586 institutions (30%) were affiliated with USA, followed by Germany (190 institutions; 10%), France (159 institutions; 8.2%), UK (138 institutions; 7.1%), and Japan (101 institutions; 5.2%). The good performance of these countries by institutions echoed the country's publication performances.

Table 3 presents the characteristics of the top 20 productive institutions using five indicators: *TP*, *SP*, *CP*, *FP*, and *RP*. No institution's ranks stayed the same by different indicators. The distribution of institution ranks was similar, but showed some variation. Except the 5th position University of Cambridge originated from UK, the other top 19 institutions were all from the USA. The top five institutions including University of California, with 125 articles, Harvard University, with 122 articles, Massachusetts Institution of Technology, with 117 articles, Stanford University, with 106 articles, and University of Cambridge with 103 articles led the list. The 9th place Yale University only ranked 32nd in *RP*, which indicating that scientists who supervised the study were less when inter-institutional collaboration was conducted. The 15th position University of Minnesota ranked 12th in *FP* and 10th in *RP*, which suggesting that the university contributed more in the collaboration. Princeton University and University of California, Santa Barbara with the highest inter-institutional collaboration rates greater than 70% had the lower ranks of 24th and 27th in *SP*. University of Illinois and University of California, San Francisco with the lowest inter-institutional collaboration rates less than 50% had the higher ranks of 7th and 7th in *SP*.

Table 3. Characteristics of the top 20 productive institutions using *TP*, *SP*, *CP*, *FP*, and *RP*

Institution	TP	*TP* R (%)	*SP* R (%)	*CP* R (%)	*FP* R (%)	*RP* R (%)	C%
University of California, USA	125	1 (2.6)	2 (1.8)	2 (3.8)	1 (2.0)	2 (1.6)	61
Harvard University, USA	122	2 (2.6)	4 (1.6)	1 (3.9)	2 (1.7)	3 (1.5)	64
Massachusetts Institution of Technology, USA	117	3 (2.5)	3 (1.7)	3 (3.5)	3 (1.7)	5 (1.4)	60
Stanford University, USA	106	4 (2.2)	1 (1.8)	6 (2.8)	4 (1.6)	4 (1.5)	53
University of Cambridge, UK	103	5 (2.2)	5 (1.5)	5 (3.1)	5 (1.4)	1 (1.6)	60
California Institution of Technology, USA	85	6 (1.8)	6 (1.4)	7 (2.3)	6 (1.4)	6 (1.3)	54
Princeton University, USA	84	7 (1.8)	24 (0.70)	4 (3.2)	8 (1.1)	7 (1.3)	77
Cornell University, USA	70	8 (1.5)	17 (1.0)	9 (2.2)	10 (1.1)	8 (1.1)	63
Yale University, USA	68	9 (1.4)	7 (1.4)	18 (1.5)	7 (1.2)	32 (0.51)	44
University of Illinois, USA	68	9 (1.4)	14 (1.0)	10 (2.0)	13 (0.93)	10 (1.0)	59
Johns Hopkins University, USA	65	11 (1.4)	11 (1.2)	13 (1.6)	11 (1.0)	12 (0.90)	51
University of Washington, USA	65	11 (1.4)	13 (1.1)	11 (1.8)	16 (0.83)	13 (0.87)	55
University of California, San Francisco, USA	63	13 (1.3)	7 (1.4)	29 (1.2)	9 (1.1)	15 (0.84)	40
University of California, Santa Barbara, USA	63	13 (1.3)	27 (0.66)	8 (2.2)	24 (0.74)	9 (1.0)	71
University of Minnesota, USA	61	15 (1.3)	12 (1.1)	18 (1.5)	12 (1.0)	10 (1.0)	49
University of Chicago, USA	57	16 (1.2)	18 (0.89)	13 (1.6)	14 (0.85)	18 (0.76)	58
University of Maryland, USA	55	17 (1.2)	24 (0.70)	11 (1.8)	22 (0.76)	16 (0.79)	65
University of California, Los Angeles, USA	54	18 (1.1)	20 (0.81)	16 (1.6)	20 (0.78)	22 (0.62)	59
Columbia University, USA	54	18 (1.1)	20 (0.81)	16 (1.6)	18 (0.80)	27 (0.56)	59
University of Pennsylvania, USA	53	20 (1.1)	19 (0.85)	18 (1.5)	20 (0.78)	22 (0.62)	57

3.1.5. Authors' Publication Performances

The author listed in one publication could be considered as the evidence of contribution [57]. The results of author analysis identified the main contributors. Among the 12,653 authors contributing to 5,320 top cited articles, 10,234 (81%) authors published one top cited article; 2,390 (19%) published 2–10 articles; 19 (0.15%) authors published 11–15 articles; and only 11 (0.087%) authors published more than 15 articles. Table 4 lists the top 11 honorary authors using *TP*, *FP*, *RP*, and *CPP*. Citations per publication (*CPP*) is obtained by dividing the total citations received during a certain period over their total publications [58]. All the honorary authors had more corresponding author articles than first author articles, and worked in the field of thermodynamics for a long time of 28 years on average.

The top three authors who contributed more to thermodynamics were K.S. Pitzer (*TP* = 38), P.J. Flory (*TP* = 31), and P.A. Kollman (*TP* = 31). The 1st place K.S. Pitzer (1914-1997) had been studying on thermodynamics for a long time of 58 years, with the first article with TC2011 $\geq$ 100 in 1937. Pitzer was a world leader in chemistry and was memorized in some papers, such as "Memorial Tribute Kenneth Sanborn Pitzer 1914–1997" [59] and "Kenneth S. Pitzer—Chemistry and Leadership" [60]. Pitzer dealt with the thermodynamic properties of concentrated solutions of

Table 4. Characteristics of the top 11 authors using *TP*, *FP*, *RP*, and *CPP*

Authors	Rank (*TP*)	Rank (*FP*)	Rank (*RP*)	CPP	PY[b] (Range)
Pitzer, KS	1 (38)	2 (19)	3 (8)	352	58 (1937-1994)
Flory, PJ	2 (31)	1 (20)	3 (8)	337	38 (1944-1981)
Kollman, PA	2 (31)	N/A[a]	1 (9)	290	16 (1987-2002)
Karplus, M	4 (25)	665 (1)	1 (9)	215	27 (1981-2007)
Fersht, AR	5 (22)	84 (3)	9 (7)	190	16 (1987-2002)
Freire, E	6 (20)	665 (1)	66 (3)	160	22 (1981-2002)
Warshel, A	7 (19)	665 (1)	18 (5)	183	18 (1986-2003)
Scheraga, HA	8 (18)	N/A[a]	32 (4)	355	52 (1954-2005)
Turner, DH	8 (18)	N/A[a]	66 (3)	240	24 (1981-2004)
Brooks, CL	10 (16)	665 (1)	18 (5)	149	18 (1987-2004)
Honig, B	10 (16)	665 (1)	32 (4)	510	14 (1989-2002)

[a]Not available. [b]Number of year from the first top cited article to the last top cited article in thermodynamics.

salts, acids, and bases [61]. Pitzer published a series of articles from no. 1 to no. 13 on the thermodynamics of electrolytes from 1973 to 1999. The first of his many papers on ion-interaction model was titled "Thermodynamics of Electrolytes. I. Theoretical Basis and General Equations" [62], also as his highest cited paper (*TC2011* = 2,043). It is now more commonly known as the Pitzer equation [59]. The Pitzer equation is now mainly used to analyze and predict the thermodynamics of electrolyte solutions over a broad range of concentration and temperature [61]. The 2nd position P.J. Flory (1910–1985), the founder of polymer science, won a Nobel Prize in Chemistry 1974 "for his fundamental achievements, both theoretical and experimental, in the physical chemistry of the macromolecules" (http://www.nobelprize.org/nobel_prizes/chemistry/laureates/1974/). Flory published the highest cited article "Thermodynamics of High Polymer Solutions" (*TC2011* = 2,125) in 1942, which was usually called Flory–Huggins theory [63]. The Flory–Huggins theory has been used in describing thermodynamics of polymer solutions [14, 63] and is still attractive now [64]. In addition, four top cited articles of a series on thermodynamics of polymer solutions was published by Eichinge and Flory in 1968, and six top cited articles of a series on statistical thermodynamics of mixtures of rod-like particles were published by Flory, Abe and Frost in 1978. The 3d ranking P.A. Kollman (1944–2001) was famous in computational chemistry and was honored in certain journals, such as "a tribute to Peter Kollman–Editor's corner" in *Proteins-Structure Function and Genetics* [65]. Kollman was the 11th most cited chemist in 1981–1997. Kollman won the American Chemical Society Computers in Chemistry Award in 1995 [66]. Two of his articles were cited over 1,000 times. One was "A Well-Behaved Electrostatic Potential Based Method Using Charge Restraints for Deriving Atomic Charges—the Resp Model" (*TC2011* = 1,796) in *Journal of Physical Chemistry* in 1993; and the other one was "The Weighted Histogram Analysis Method for Free-Energy Calculations on Biomolecules. 1. The Method" (*TC2011* = 1,260) in *Journal of Computational Chemistry* in 1992, for the weighted histogram analysis method (WHAM).

The 4th M. Karplus from Harvard University published 25 top cited articles from 1981 to 2007. Karplus had the *CPP* of 215, and two articles cited more than 500 times. One was "How Does a Protein Fold" (*TC2011* = 679) in *Nature* in 1994, and the other one was "Simulation of Activation Free Energies in Molecular Systems" (*TC2011* = 524) in *Journal of Chemical Physics* in 1996. Karplus and his group contributed to the development of molecular dynamics and Monte Carlo simulation technique (http://www.chem.harvard.edu/research/faculty/martin_karplus.php). The 5th A.R. Fersht from University of Cambridge published 22 top cited articles from 1987 to 2002. The most cited article of him was "Folding of Chymotrypsin Inhibitor-2. 1. Evidence; for a 2-State Transition" (*TC2011* = 624) with Jackson in *Biochemistry* in 1991. The 6th E. Freire from Johns Hopkins University published

20 top cited articles in 1981–2002. The most cited article of Freire was "HIV-1 Evades Antibody-Mediated Neutralization through Conformational Masking of Receptor-Binding Sites" (*TC2011* = 377) in *Nature*. Freire laboratory's research resulted in the development of a thermodynamic platform for drug discovery and optimization (http://www.bio.jhu.edu/Faculty/Freire/). The 7th place A. Warshel from University of Southern California published 19 top cited articles from 1986 to 2003. Warshel published "Microscopic and Semimicroscopic Calculations of Electrostatic Energies in Proteins by the Polaris and Enzymix Programs" (*TC2011* = 318) in *Journal of Computational Chemistry* received the most citations. The 8th position H.A. Scheraga from Cornell University and D.H. Turner from Columbia University both published 18 top cited articles in the longest period of 52 years from 1981 to 2002 and from 1984 to 2004, respectively. The high *CPP* of 355 for Scheraga was due to his three top articles with more than 1,000 *TC2011*. These three articles made a series on structure of water and hydrophobic bonding in proteins by Nemethy and Scheraga in 1962. Turner had the *CPP* of 240, and the most heavily cited article was "Improved Free-Energy Parameters for Predictions of RNA Duplex Stability" (*TC2011* = 1,175) in *Proceedings of the National Academy of Sciences of the United States of America*. The 10th place C.L. Brooks from the University of Michigan and B. Honig from Columbia University both had 16 top cited articles in 1987–2004 and 1989–2002, respectively. Brook's topmost article was published in Science, titled "First-Principles Calculation of the Folding Free-Energy of a 3-Helix Bundle Protein" (*TC2011* = 309). Brooks group's current interests include free energy based methods for inhibitor screening and optimization, including lambda-dynamics, ligand docking, protein stability and continuum based free energy approximations (http://brooks.chem.lsa.umich.edu/). In particular, Honig had the highest *CPP* of 510, which is attribute to his most highly cited article, had *TC2011* of 5,006, which presented a widely used software GRASP [67]. Honig group has focused on the development and application of biophysical and bioinformatics methods aimed at understanding the structural and energetic origins of protein-protein, protein-nucleic acid, and protein-membrane interactions (http://wiki.c2b2.columbia.edu/honiglab_public/index.php/Main_Page). Among these top authors, only the 2nd place P.J. Flory won the Nobel Prize with 337 citations per top cited article. It is believed that Nobelists are consistently highly cited while only a small percentage of top cited authors win the prize [68].

3.2. Top Articles in the History and in the Latest Year

3.2.1. Top Articles with the Highest *TC2011*

Although the indicator of total citations is popularly to judge the level of one publication [69], this indicator was too rough to recognize the impact of articles. Citation life cycles of top articles were examined to look further and deeper into the performance of them [32, 70]. The articles with the highest *TC2011* can be considered the most popular players in the past 110 years. The citation lives of the top five articles (*TC2011* > 4,000) were shown in Fig. 5. The article published by Wigner [13] in 1932 was the earliest article. The other four articles (Nicholls et al. (1991), Delaglio et al. (1995), Kresse and Furthmüller (1996), and Scott and Radom (1996)), which were all published after 1990, had a relatively short time span for citations. The new players in the 1990s stepped into the top five according to *TC2011*, which indicating that they received citations quicker. All curves of the citation life cycles were uneven. These top articles accumulated their citations in different patterns of citation life cycles. Some of the top players still received high citations in recent years, such as Wigner (1932), but some of them received low citations, such as Nicholls et al. (1991). The citation pattern of top cited articles varied from article to article. Pronounced differences of the life cycle curves among publications were not surprising since distinct citation patterns have ever identified and classified in other disciplines [70, 71].

The 1st and 2nd position Kresse and Furthmüller (1996) and Delaglio et al. (1995) with high *TC2011* also had high citation in recent years. Only two of them: Kresse and Furthmüller (1996) and Delaglio et al. (1995), saw sharply increasing trends and rose to the maximum 1,324 and 583 in 2011 since publication. Kresse and Furthmüller (1996) received very high citations of 531 per year on average since 1996, and still obtained 1,324 citations in 2011, affecting a large number of studies. Kresse and Furthmüller [15] presented a detailed description and comparison of algorithms for performing AB-initio quantum-mechanical calculations using pseudopotentials and a plane-wave basis set. In this article, Vienna AB-initio molecular-dynamics package (VAMP) had been used successfully for a large number

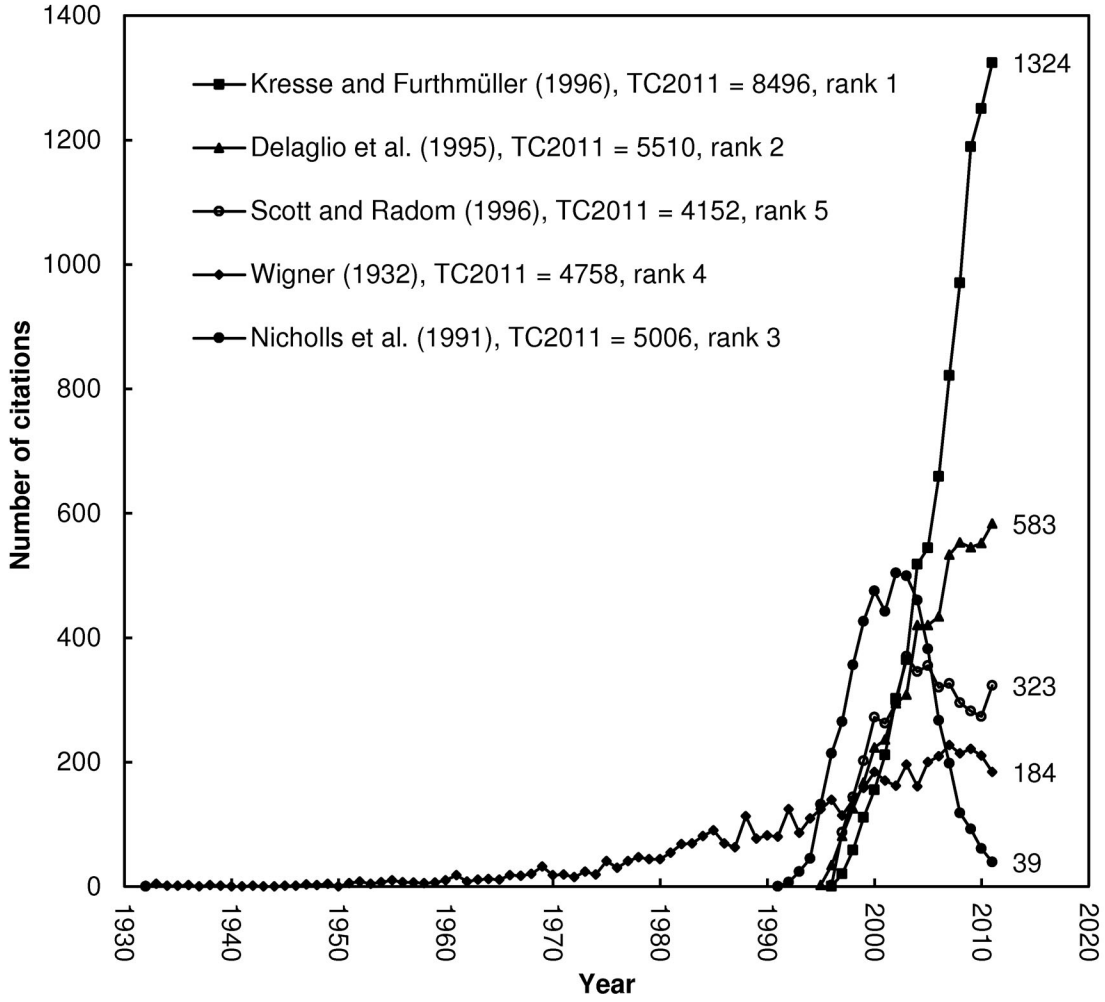

Fig. 5. Citation life cycles of the top five articles (*TC2011* > 4,000).

of different systems. Moreover, Kresse and his coworkers conducted many works to develop Vienna AB initio simulation package (VASP) [72–74]. The 2nd position player, Delaglio et al. (1995) also had a high growth rate. Delaglio, Grzesiek, Vuister, Zhu, Pfeifer and Bax [75] presented the NMRPipe system, a comprehensive new multidimensional spectral processing via UNIX pipes. It is a UNIX software environment of processing, graphics, and analysis tools designed to meet current routine and research-oriented multidimensional processing requirements, and to anticipate and accommodate future demands and developments [75]. The information of NMRPipe was included in the Software list of Bax group (http://spin.niddk.nih.gov/bax/).

Both Scott and Radom (1996) and Wigner (1932) experienced quick increase, and went into the phase without obvious uptrends in last decade. Scott and Radom [76] worked to determine optimum frequency scale factors suitable for the prediction of vibrational fundamentals, low-frequency vibrations, zero-point vibrational energies, and thermal contributions to enthalpy and entropy, from calculated harmonic vibrational frequencies. Radom and his co-workers also attempted to evaluate frequency scale factors suitable for the prediction [77]. Wigner (1932), the earliest player, first had been cited a few times (257; 6.2%) in a long time from 1932 to 1970, and then started to obtain citations quicker, especially in the 1990s. Wigner [13] developed a formula for a correction by means of a probability function in thermodynamic equilibrium. This function was usually called Wigner function [78]. The Wigner function is particularly appropriate as a "quantum phase-space distribution" for describing the effects on the quadrature observables that may arise from quantum theory and classical statistics [79]. The classic early article has had a strong and lengthy influence on the thermodynamic field.

Particularly, the 3d position Nicholls et al. (1991) with *TC2011* = 5,006 had a low visibility of 39 citations in 2011, ranking 336th based on *C*2011. Citations of Nicholls et al. (1991) initially climbed from zero in 1991 to peak of 504 in 2002 and then decreased to only 39 in 2011. Nicholls, Sharp, and Honig [67] demonstrated that the surface tension, water-organic solvent, transfer-free energies and the thermodynamics of melting of linear alkanes provide fundamental insights into the nonpolar driving forces for protein folding and protein binding reactions. GRASP is a graphics program that is widely used by the structural biology community to visualize macromolecules, available at http://wiki.c2b2.columbia.edu/honiglab_public/index.php/Software:GRASP. Honig group encouraged researchers to list article Nicholls et al. as a reference in all articles that use GRASP. The widespread use of the original version of GRASP demonstrated the importance of the visualization of physicochemical and structural properties on the molecular surface [67]. A new version, GRASP2, is an updated version of the GRASP program used for macromolecular structure and surface visualization [80]. This article related to GRASP2 was published in 2003, just the time of first year of the drop of received citations of Nicholls et al. (1991). The issue of this new version may be the reason of the turning point of decline. One possible reason for a sudden decline of the top cited article was the replacement of a new method.

3.2.1. Top Articles with the Highest *C*2011

Only the *TC2011* used was not enough to identify some excellent articles in the most recent years. Some recent articles, which did not get enough time to accumulate citations, would be omitted if only *TC2011* was employed for evaluation. For example, the 101st position Phillips et al. (2006) (*TC2011* = 856) with a high *C*2011 of 308 would not be prominent if only *TC2011* was considered. Total number

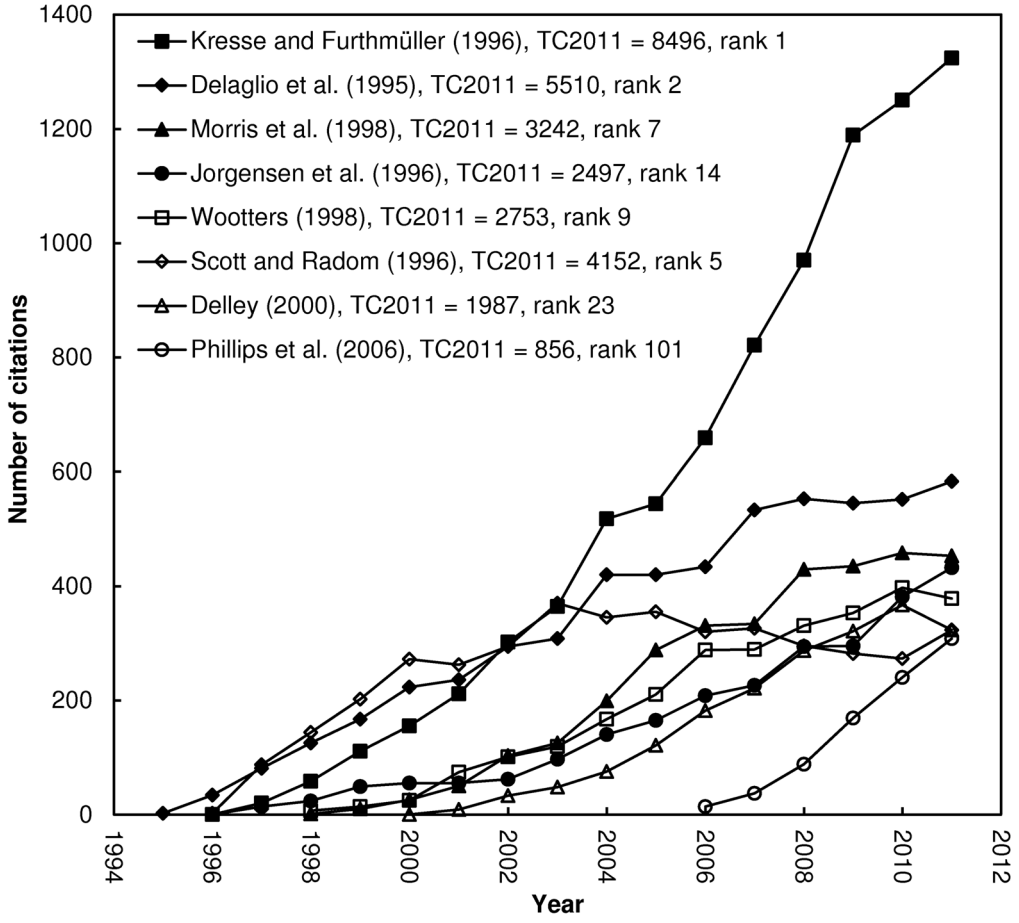

Fig. 6. Citation life cycles of the top eight articles (*C*2011 > 300).

of citations of a paper in the latest year (2011) was recorded as $C2011$. Figure 6 exhibits the citation history of the top eight articles which had $C2011 > 300$. As expected, these articles all had high annual citation growth rates, presenting great vigor and vitality. Three articles of Kresse and Furthmüller (1996), Delaglio et al. (1995), and Scott and Radom (1996), which had both $TC2011 > 4{,}000$ and $C2011 > 300$, overlap in Figs. 5 and 6. These three well-known articles had a strong and long influence on the thermodynamics field. All the articles emerged in the 1990s and the 2000s, while no articles published before 1990 still maintain high visibility in 2011. The field thermodynamics was lively with the most influential articles in recent years.

The 3d Morris et al., 4th Jorgensen et al., and 5th Wootters by $C2011$ were all published in the 1990s. Morris, Goodsell, Halliday, Huey, Hart, Belew, and Olson [81] developed and tested a novel and robust automated docking method that predicts the bound conformations of flexible ligands to macromolecular targets has been developed and tested, in combination with a new scoring function that estimates the free energy change upon binding. The new search methods and empirical free energy function are available in AutoDock 3.0 [81]. Olson and his collaborator had developed AutoDock 1 [82], AutoDock 2.4 [83], and AutoDock 4 Scoring Function [84] after. The detailed information about AutoDock was found on Olson Laboratory Web available at http://mgl.scripps.edu/. AutoDock is the most commonly cited docking program in the scientific literature [85]. Jorgensen, Maxwell, and TiradoRives [86] described the development and testing of the OPLS all-atom force field. Both nonbonded and torsional energy parameters were derived to reproduce gas-phase structures and conformational energetics and observed thermodynamic properties of organic liquids [86]. Jorgensen and his co-workers also examined the OPLS all-atom force field for carbohydrates [87] and heterocycles [88]. The Jorgensen Research group has been worked on the forefront of computational chemistry and molecular design for the past thirty years (http://zarbi.chem.yale.edu/). Wootters [89] worked on entanglement of formation of an arbitrary state of two qubits. Wootters has studied the quantum information theory for nearly thirty years [90], and tried to find quantitative rules governing the entanglement between two or more quantum objects more recently [91].

Delley (2000) and Phillips et al. (2006) in the 2000s had strong influence in recent years. Delley [92] described recent extensions of the DMol^3 local orbital density functional method for band structure calculations of insulating and metallic solids. Delley contributed to the development of computer codes for density functional theory DMol^3 [92, 93]. The latest article Phillips et al. (2006) had a high grow rate of 59 citations per year. Phillips, Anderson, and Schapire [94] introduced the use of the maximum entropy method (Maxent) for modeling species geographic distributions with presence-only data. Maxent is a general-purpose machine learning method with a simple and precise mathematical formulation, and it has a number of aspects that make it well-suited for species distribution modeling [94]. Phillips conducted much work on Maxent in recent years [95, 96].

4. CONCLUSIONS

The characteristics of languages, publication outputs of decades, journals, Web of Science categories, countries, institutions, authors, and top articles with exceptionally high $TC2011$ and $C2011$ were revealed. Firstly, the 5,320 top cited articles received a mean number of 210 citations over the last 109 years from 1902 to 2010, with more than three fifths of the articles published after 1990. Secondly, 686 journals were represented, led by *Journal of the American Chemical Society*, *Journal of Chemical Physics* and *Physical Review Letters*. Multidisciplinary chemistry, biochemistry and molecular biology, and physical chemistry led the 130 Web of Science categories. Thirdly, 1,936 institutions from 63 countries/territories contributed to the articles. Harvard University, Massachusetts Institution of Technology, and University of Washington in the USA were the three most productive institutions. The eight major industrialized countries G8 accounted for 87% of total articles, the USA for 61%, and more international collaboration was involved than the general norm. Moreover, K.S. Pitzer, P.J. Flory, and P.A. Kollman contributed a lot to the development of thermodynamic research with Pitzer equation, Flory–Huggins theory, and weighted histogram analysis method. Finally, the citation patterns as a function of time varied widely among the top articles. Wigner function in one early classical article has been frequently cited and still has a strong influence. Frequency scale factors, OPLS all-atom force field, entanglement between two or more quantum objects, and some softwares including VAMP, NMRPipe, GRASP2, AutoDock, DMol^3, and Maxent have experienced a high growth rate of citations. The development of thermodynamics involved many parallel computing and software.

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