Intellectual Authorities and Hubs of Green Chemistry

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Abstract. Green Chemistry (GC) is an answer to the problems ensuing from chemical pollution, adopting a proactive, prevention-based stance. After nearly three decades of its coming into being, the advances in the field towards groundbreaking chemical practice are still under discussion and new research is needed in order to systematize existing knowledge and to point to efficient means to select information. Our purpose with this study is to broaden the understanding on GC research structure, by pointing the researchers that have most contributed to its growth, spread and consolidation (its intellectual hubs), and the authors upon whose knowledge they have drawn (intellectual authorities). We analyzed 14,142 documents either containing the term "green chemistry" or published in *Green Chemistry* and *Green Chemistry Letters and Reviews* between 1990 and 2017, using network analysis and co-citation analysis. Fourteen hubs were found, and twenty-one intellectual authorities, distributed along six big specialties, previously described in the literature. Results corroborate previous analyses of the field, but this research has the advantage of stemming from the dynamics of scientific production, rather than from previously defined qualitative categories of the field itself.

Keywords: Green Chemistry · Co-citation analysis · CiteSpace

1 Introduction

There is currently a worldwide concern with preserving the environment and drastically reducing global warming. Chemistry seems to be a key agent in the current state of affairs, as it may be one of the most important sciences contributing to either aggravate or completely solve the problem. A solution within the scientific community has been growing since 1990 [1, 2], the so-called *Green Chemistry* (GC). The number of papers advocating CG-based solutions went from n = 133 (1999) to n = 3,093 (2018), a growth of more than 2,000% in two decades, as research on the Web of Science shows.

GC appears as a response to the limits of pollution and risk control policy (retroactive measures) [3], adopting a proactive, prevention-based approach. In the wake of the Pollution Prevention Act [4], GC's strategy is to reduce the use and disposal of hazardous substances, by establishing twelve principles for a green practice [5]: (1) Waste

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Prevention; (2) Atom Economy; (3) Less Hazardous Chemical Synthesis; (4) Designing Safer Chemicals; (5) Safer Solvents and Auxiliaries; (6) Design for Energy Efficiency; (7) Use of Renewable Feedstocks; (8) Reduce Derivatives; (9) Catalysis; (10) Design for Degradation; (11) Real Time Pollution Prevention; and (12) Inherently Safer Chemistry for Accident Prevention.

Almost three decades after GC was created, the advances of the field for groundbreaking chemical practice are still under discussion, usually from the perspective of its principles [2, 8–10]. Recent studies [6, 7] have detached themselves from the Twelve Principles, and sought research topics emerging from co-citation analysis of the papers published in the field, finding six main lines of research (*big specialties*) organized around sixteen smaller thematic groups, called *research specialities* (Table 1).

Table 1. Specialties in GC research. Adapted from Marcelino, Pinto and Marques [6] and Marcelino and Marques [7].

Big speciality	Research specialties
A-Solvents	#4 – Organic Reaction in Aqueous Media
	#5 – Supercritical Solvents
	#17 – Deep Eutectic Solvents
	#18 – Organic Reaction in Aqueous Media
B-Ionic Liquids	#0 – Ionic Liquids
	#6 – Recycling and Recovery of Solvents
	#8 – IL Toxicity
	#12 – IL Preparation
C-Biomass	#3 – Biomass Transformation
	#11 – Lignin Valorization
	#16 - Glycochemistry
D-Catalysis	#2 – Metal Catalysis and Microwave Activation
	#9 – Solid Acid Catalysis
	#10 – Catalytic Oxidation of Alcohols
E – GC Characterization	
F – CO_2 as Substrate	

Each specialty is conceptualized and visualized as the relationship between a time-variant network $\Phi(t)$ of co-cited papers (its intellectual base $\Omega(t)$) and the papers that promote co-citations in the network (its research front $\Psi(t)$) [11, 12], as presented in Eq. (1).

$$F(t) : Y(t) \rightarrow W(t) \tag{1}$$

Taking into account GC's potential for an environmentally benign chemical practice in the current context of the environmental crisis, research is needed that systematizes

the knowledge already produced, and points to more effective means of selecting information. The above-mentioned study [6] presents a broad overview of GC research, and provides important information on the structure and relationship between specialties, thus helping researchers in the field trace relevant information for their researches more efficiently. Our purpose with this research is to broaden the understanding on GC research structure, by pointing the researchers that have most contributed to its growth, spread and consolidation (its intellectual hubs), and the authors upon whose knowledge they have drawn (intellectual authorities).

Section 2 discusses the concepts of *hubs* and *intellectual authorities* in the context of the specialties defined around an intellectual base and a research front. Section 3 details methodology. Section 4 presents the hubs and intellectual authorities for each of GC's big specialties (4.1 Intellectual Hubs and Authorities of GC Specialties) and validates the data based on prior discussions in the literature (4.3 Results validation). Finally, we present the conclusions and references. The complete table with the research data can be accessed in the Supplementary Material[1].

2 Hubs and Intellectual Authorities

Jon Kleinberg [13] has developed an algorithm to analyze the importance of network nodes in providing content of relevance (authorities) or the ability to select, group and disseminate information (hubs). Kleinberg's algorithm is based on mutual recursion, so that, in a given network, an important hub connects to important authorities, and vice versa.

In the case of the present study, we have a structured co-citation network with an intellectual base (cited papers) and information on the research fronts, the papers that cite the works of this network [11, 12]. This would mean that there is an invisible network formed by the research front that interacts with the visible network made by the intellectual base. By considering these two sources of information, we have made Kleinberg's analysis of hubs and authorities more complex, and developed an alternative thereto.

We consider that certain authors within the research front act *as* hubs: nodes with high degree of connection, grouping the intellectual base around a research theme and disseminating information throughout the scientific community. We have two indicators of hub behavior of a research front paper: its Coverage (Cov) value and Global Citation Score (GCS). Coverage gives us the concentration intensity, how much a certain author contributes to grouping information and shaping a research/specialty front. It is a measure associated with the author's contribution to tie research around a specific theme. The GCS is the amount of citations a given paper has received within the scientific community, and provides an idea of the role of the researcher in provoking the diffusion of the research/specialty front or how much it has been disseminated within the Chemistry community.

Some authors of the intellectual base act *as* authorities: nodes with relevant information that are linked by several dissemination nodes, the hubs. Intellectual authorities

[1] http://bit.do/ESM_husbs-authorities.

provide the concepts, methodologies and techniques necessary for the existence of a specialty. There are three indicators defined by Chen [11, 12] that we used for identifying intellectual authorities: citation frequency (CF), citation burstness (CB), and betweenness centrality (BtC). CF measures how many times the author was cited within the selected sample, which can be called the *Local Citation Score* (LCS). Unlike GCS, which considers all citations of a given piece of work in all the literature, CF is an indicator of the recognition of the paper/author by green chemists (a group of previously selected works), which allows us to draw inferences on the recognition of a given specialty. CB measures a sudden increase in the number of citations to a document/author, and is an indicator of the degree of innovation introduced in the field of knowledge, which generates sudden interest in a given subject. BtC is the ability of a work/author to transit among various specialties, promoting interaction and information exchange. These elements with high BtC fill gaps in the structure of knowledge and act as bridges among different research topics.

To find these hubs and authorities, we consider several metrics, adding the values of each author's output to reach a total. For a given author, LCS, number of papers (NP), CF, BtC and CB values are all calculated by the simple sum of the individual values of each metric for an author's papers. Total GCS is the sum of GCS values of different papers by an author. Nevertheless, a given authors' total coverage is measured by the quotient of the number of papers this author cites in the intellectual base by the total number of papers in the intellectual base of a specialty.

3 Methodology

All data were collected in May 2018 in the Web of Science database (Core Collection, indexes: SCI-EXPANDED, SSCI, A&HCI, CPCI-S, CPCI-SSH, ESCI) from 1990 (the decade in which GC emerges [1, 2]) to 2017 (he last full year at the time of analysis). We selected documents containing references, such as: papers, reviews, proceedings papers and book chapters (henceforth *papers*). We searched for the term "green chemistry" in titles, keywords and abstracts, thus indicating explicit affiliation to GC. We also selected all texts published in *Green Chemistry Journal* and *Green Chemistry Letters and Reviews*, as these are GC journals, and their texts do not always use the descriptor "green chemistry" in their titles, abstracts and keywords.

We obtained a final set of 14,142 different records (duplicates excluded), being 8,586 records with the term "green chemistry" and 6,004 in specialized journals. We analyzed this data using CiteSpace (version 5.2.R1.3.9.2018), considering: Look Back Year (LBY): −1; Time Slice: 3 years (1990–2017); Node types: Cited reference; Top N.: 100. These parameters were chosen for their best results in Modularity Q and Silhouette values. Other parameters followed default program settings. After the network was created, the algorithm was applied for the generation of clusters, the themes of which were inferred from the titles and abstracts of the papers in the research front of each cluster. The authors names were standardize to avoid duplicates, specially the given names that were fully abbreviated without punctuations and spaces.

The validation of the analysis is made by considering the internal evaluation parameters of the network (Modularity Q and silhouette) and peer recognition (comparison

with previous qualitative description of the field made by renowned researchers) [2, 14], important criteria for validation, as Noyons [15] points out.

4 Results and Discussion

4.1 Intellectual Hubs and Authorities of GC Specialties

A – Solvents. The analysis of the authors who contribute the most to the dissemination and consolidation of a specialty (its intellectual hubs) may be done by means of the coverage value that they accumulate in a big specialty, that is, by the proportion of papers co-cited by a text/author, given the total amount of papers cited in the intellectual base of the specialty or big especialty (BSp).

Big specialty A – Solvents has 43 papers in its research front, among which Victorio Cadierno and Javier Franco have the highest coverage values (0.24 and 0.18 respectively) and also the highest number of papers (Table 2). The next ten authors are all related to the same paper in the research front of small specialty #5 – Supercritical Solvents. As this front is composed of only two papers, its coverage is high. Pascale Crochet occupies the third position in number of papers, with 3 texts in A – Solvents, and an accumulated coverage of 0.14. Paul T. Anastas, Nicolas Eghbali, Vivek Polshettiwar and Rajender S. Varma possess the highest citation values, but do not have high coverage values, meaning that they have papers acknowledged by the scientific community as a whole, but they are not necessarily the ones most closely related with A – Solvents. Cadierno, Franco and Crochet, however, have a GCS of approximately 200, and follow the highest-ranking authors in this indicator.

With regard to the intellectual authorities present in the intellectual base (72 papers) of big specialty A – Solvents (Table 3), Chao-Jun Li has the largest number of papers used in the references of the research front, with a high accumulated CF of 951, almost three times as big as the runner-up (Varma, 85). Li stands out in terms of CB, with twice as many citations (117) as the second place (Abbott, 46), meaning that his works were especially important for this specialty, approaching subjects that aroused the interest of its researchers. CB for the output of this intellectual base occurs, on average, between 2006 and 2009, which is neither as old as the average CB of B – Ionic Liquids (2003–2006), nor as new as the average CB of C – Biomass (2011–2014).

Li also has the highest accumulated BtC, meaning that his works in this specialty possibly interact with other specialties, strengthening the field of GC as a whole. It should be pointed out that both A – Solvents and C – Biomass are big specialities with the lowest accumulated BtC values per author, meaning that, even though their authorities promote interaction throughout GC, their reach is more limited. Mark J. Burk e William D. McGhee have a high number of papers on the intellectual base, but these have low CF or CB, which indicates that they did not generate much interest in the community, even if they are important for this big specialty.

We may, therefore, conclude that Victorio Cadierno and Javier Franco are the leading authors in terms of output and contributions to co-citations in the research fronts of big specialty A – Solvents, and may be considered its intellectual hubs. Chao-Jun Li is the author with the highest number of papers in the intellectual base, accumulating the highest CF, CB and BtC, demonstrating his importance in providing support to the works

Table 2. Big specialty A – Solvents, most relevant authors of the research front.

Author	Cov A	Total Cov	GCS A	Total GCS	LCS A	Total LCS	N BSp
CADIERNO, V	0.2411	0.0527	245	397	5	7	2
FRANCOS, J	0.1851	0.0417	200	352	4	6	2
BORKOWSKY, SL	0.1667	0.0327	79	79	1	1	1
BROWN, GH	0.1667	0.0327	79	79	1	1	1
BURK, MJ	0.1667	0.0327	79	79	1	1	1
FENG, S	0.1667	0.0327	79	79	1	1	1
GROSS, MF	0.1667	0.0327	79	79	1	1	1
LELACHEUR, RM	0.1667	0.0327	79	79	1	1	1
LUAN, L	0.1667	0.0327	79	79	1	1	1
MORGENSTERN, DA	0.1667	0.0327	79	79	1	1	1
MORITA, DK	0.1667	0.0327	79	79	1	1	1
TUMAS, W	0.1667	0.0327	79	79	1	1	1
CROCHET, P	0.1421	0.0409	197	393	3	7	4
JIANG, B	0.0990	0.0194	175	175	2	2	1
LI, GG	0.0990	0.0194	175	175	2	2	1

in big specialty A – Solvents, acting as an intellectual authority for these studies. Within this big specialty, it is important to highlight the importance of the research in organic reactions in aqueous medium (cluster #18), as it is one of its most recognized subjects of study, and has the largest research front.

B – Ionic Liquids. This big specialty has the second smallest research front, with 27 papers published between 1996 and 2017. Table 4 presents the most important authors of the research fronts of big specialty B – Ionic Liquids, classified in descending order of coverage. Five authors stand out with values above 0.2: Robin D. Rogers, John D. Holbrey, W. Matthew Reichert, Richard P. Swatloski and Kenneth R. Seddon. All five of them have a large number of papers concentrated in the research front of this big specialty, in particular Rogers and Seddon, with four papers each. Seddon also stands out in the number of citations accumulated by his papers, with 1,240, followed by Louis C. Branco, João N. Rosa, Joaquim J. M. Ramos e Carlos A. M. Alfonso, who accumulated 948 citations of their papers.

The intellectual base of this big specialty has 112 papers, the largest of them all, with papers published between 1973 and 2011. Due to the size of the intellectual base, there is a large number of papers published by the authors (Table 5): Kenneth R. Seddon has 17 papers, all within this great specialty, showing his dedication and contribution to the theme. Other authors with a large number of publications include Robin D. Rogers, John D. Holbrey, Tomas Welton, Richard P. Swatloski and Peter Wasserscheid. Four of these authors stand out due to the high CF and CB accumulated by their works, demonstrating the interest that their studies have raised for research on ionic liquids: Welton has the

Table 3. Big specialty A – Solvents, most relevant authors of the intellectual base.

Authors	NP A	Total NP	N BSp	CB A	Total CB	BtC A	Total BtC	CF A	Total CF
LI, CJ	10	9	2	117.46	133.09	0.17	0.2	951	1074
VARMA, RS	9	2	2	32.11	118.59	0.05	0.21	85	426
JESSOP, PG	6	2	4	12.04	89.5	0.09	0.32	20	279
BURK, MJ	4	4	1	5.25	5.25	0.09	0.09	14	14
MCGHEE, WD	4	4	1	0	0	0.01	0.01	9	9
DESIMONE, JM	4	3	2	4.59	18.79	0.01	0.01	11	107
CHAN, TH	3	3	1	44.42	44.42	0.02	0.02	194	194
IKARIYA, T	3	2	2	12.04	33.2	0.09	0.13	20	57
NOYORI, R	3	2	2	12.04	33.2	0.09	0.13	20	57
JEROME, F	3	1	3	28.21	63.23	0.01	0.2	87	180
TUMAS, W	3	1	3	5.25	21.7	0.09	0.09	8	108
BRESLOW, R	2	2	1	19.69	19.69	0.06	0.06	89	89
ABBOTT, AP	2	2	1	46.39	46.39	0.01	0.01	128	128
DOMLING, A	2	2	1	19.66	19.66	0.02	0.02	216	216
LINDSTROM, UM	2	2	1	31.32	31.32	0.06	0.06	332	332
BIENAYMÉ, H	2	2	1	20.42	20.42	0.03	0.03	236	236
FOKIN, VV	2	2	1	24.08	24.08	0.02	0.02	358	358
FINN, MG	1	1	1	3.99	3.99	0.01	0.01	190	190
KOLB, HC	1	1	1	3.99	3.99	0.01	0.01	190	190
MULDOON, J	1	1	1	3.99	3.99	0.01	0.01	190	190
SIMON, MO	1	1	1	26.61	26.61	0.07	0.07	140	140
ROYER, S	1	1	1	28.21	28.21	0.01	0.01	87	87
VIGIER, KD	1	1	1	28.21	28.21	0.01	0.01	87	87
ZHANG, QH	1	1	1	28.21	28.21	0.01	0.01	87	87
FENG, SG	1	1	1	5.25	5.25	0.09	0.09	8	8
GROSS, MF	1	1	1	5.25	5.25	0.09	0.09	8	8
CHEN, L	1	1	1	9.16	9.16	0.02	0.02	192	192
BLACKERT, JF	1	1	1	4.01	4.01	0.1	0.1	6	6
TANKO, JM	1	1	1	4.01	4.01	0.1	0.1	6	6

highest accumulated CF value (831), followed by Seddon (774), Wasserscheid (463) and Rogers (335). Seddon, however, presents the highest CB value (2192.7), followed by

Table 4. Big specialty B – Ionic Liquids, most relevant authors of the research front.

Author	Cov B	Total Cov	GCS B	Total GCS	LCS B	Total LCS	N BSp
ROGERS, RD	0.295	0.090	612	612	4	4	1
HOLBREY, JD	0.231	0.070	584	584	3	3	1
REICHERT, WM	0.221	0.067	594	594	3	3	1
SWATLOSKI, RP	0.221	0.067	594	594	3	3	1
SEDDON, KR	0.201	0.061	1240	1240	4	4	1
AFONSO, CAM	0.161	0.049	948	948	2	2	1
BRANCO, LC	0.161	0.049	948	948	2	2	1
RAMOS, JJM	0.161	0.049	948	948	2	2	1
ROSA, JN	0.161	0.049	948	948	2	2	1
BROKER, GA	0.157	0.048	566	566	2	2	1
KITAZUME, T	0.142	0.046	164	187	3	4	2
VISSER, AE	0.142	0.043	169	169	2	2	1
ZULFIQAR, F	0.117	0.036	143	143	2	2	1
STOLTE, S	0.090	0.027	200	200	2	2	1
THOMING, J	0.090	0.027	200	200	2	2	1

Holbrey, Rogers and Welton with aproximately 1,000 each. Among these four authors, Seddon stands out for his accumulated BtC value (0.31), showing that his works allow for interaction among specialties.

Considering the number of papers on the research fronts and the high number of accumulated citations, we can say that Robin D. Rogers and Kenneth R. Seddon are the main intellectual hubs of big specialty B – Ionic Liquids, with great contribution to set the boundaries and spread discussions of this specialty. Other authors displaying hub behavior are John D. Holbrey, W. Matthew Reichert and Richard P. Swatloski. In the intellectual base, Kenneth R. Seddon also has great importance, as he is the most published and has the highest accumulated CB value, and second highest CF value, acting also as intellectual authority of this great specialty. Other revelant authors as intellectual authorities on ionic liquids are Robin D. Rogers, Tom Welton and Peter Wasserscheid. The recurrence of authors in the research front and intellectual base demonstrates the internal cohesion of this big specialty; additionally, the fact that this big specialty holds the highest CB values indicates the great interest and commitment that the theme has aroused among its researchers, especially until 2009.

C – Biomass. This research front is the fourth largest within GC, with 42 papers published from 1999 to 2017. The authors with the highest coverage in this specialty are David M. Alonso, James A. Dumesic and Atsushi Takagaki, all with 0.202 each, and two appearances on the research fronts (Table 6). Michikazu Hara comes third in accumulated coverage, and appears four times in the research fronts, the hightest LCS. Yan-Long Gu has the second highest LCS value, appearing three times in the research fronts, despite his

Table 5. Big specialty B – Ionic Liquids, most relevant authors of the intellectual base.

Authors	NP B	Total NP	N BSp	CB B	Total CB	BtC B	Total BtC	CF B	Total CF
SHELDON, R	23	4	5	92,15	275,84	0,06	0,5	313	1718
SEDDON, KR	17	17	1	228,41	228,41	0,31	0,31	774	774
ROGERS, RD	12	9	3	113,43	149,52	0,12	0,27	335	612
SWATLOSKI, RP	9	7	2	76,4	94,37	0,07	0,22	141	359
HOLBREY, JD	8	7	2	107.89	114.85	0,07	0,21	206	403
WELTON, T	8	7	2	136,34	152,53	0,18	0,18	831	869
JASTORFF, B	7	7	1	81,96	81,96	0,15	0,15	182	182
RANKE, J	7	7	1	81,96	81,96	0,15	0,15	182	182
VISSER, AE	6	6	1	84,45	84,45	0,11	0,11	190	190
EARLE, MJ	6	6	1	66,77	66,77	0,03	0,03	197	197
WASSERSCHEID, P	6	6	1	114.14	114.14	0,03	0,03	463	463
DE SOUZA, RF	5	5	1	58.69	58.69	0.16	0.16	288	288
DUPONT, J	5	5	1	58.69	58.69	0.16	0.16	288	288
SUAREZ, PAZ	4	4	1	58.69	58.69	0.16	0.16	284	284
DULLIUS, JEL	3	3	1	27.18	27.18	0.16	0.16	60	60
EINLOFT, S	3	3	1	27.18	27.18	0.16	0.16	60	60
KEIM, W	1	1	1	41.22	41.22	0,02	0,02	311	311
KLEMET, I	1	1	1	3.96	3.96	0.25	0.25	6	6
KNOCHEL, P	1	1	1	3.96	3.96	0.25	0.25	6	6
LUTJENS, H	1	1	1	3.96	3.96	0.25	0.25	6	6

ranking 7th in accumulated coverage, with 0.162. Alonso and Dumesic have a high GSC value, being cited 1,061 times each, but it is Joseph J. Bozell and Gene R. Petersen, who hold the highest accumulated CF value, 1,404 each, thus establishing their importance for biomass research.

The intellectual base of C – Biomass contains 49 works, published between 1993 and 2016. James A. Dumesic stands out with the highest number of papers (9), followed by George W. Huber (5) (Table 7). The high number of contributions to C – Biomass indicates that they their output grounds the discussions on these specialties. The authors with the highest accumulated CF are Avelino Corma and Sara Iborra with 717 each, followed by James A. Dumesic (661) and George W. Huber (556); these authors are the most acknowledged by the scientific community on this intellectual base. The same four authors are the ones with the highest CB value, which represents how their output has arisen the interest and commitment of research in this specialty. Dumesic's accumulated CB (1,035.5) is worthy of note, being almost twice as big as that of his runner-up

Table 6. Big specialty C – Biomass, most relevant authors of the research front.

Author	Cov C	Total Cov	GCS C	Total GCS	LCS C	Total LCS	N BSp
ALONSO, DM	0.202	0.027	1061	1061	2	2	1
DUMESIC, JA	0.202	0.027	1061	1061	2	2	1
TAKAGAKI, A	0.202	0.038	204	230	2	3	2
HARA, M	0.182	0.071	291	485	4	7	2
RENDERS, T	0.163	0.022	14	14	2	2	1
SELS, BF	0.163	0.030	14	122	2	3	2
GU, YL	0.162	0.029	378	707	3	5	3
HAYASHI, S	0.141	0.049	160	249	2	4	2
BELL, AT	0.141	0.019	233	233	1	1	1
CHIDAMBARAM, M	0.141	0.019	233	233	1	1	1
CLIMENT, MJ	0.141	0.019	413	413	1	1	1
IBORRA, S	0.141	0.019	413	413	1	1	1
CORMA, A	0.141	0.022	413	445	1	2	2
GALKIN, MV	0.122	0.016	1	1	1	1	1
KUMANIAEV, I	0.122	0.016	1	1	1	1	1

(Corma, 672,9). The average CB of C – Biomass spans from 2011 to 2014, the most recent interval, which may indicate the interest that the most recent studies have aroused in this topic and its relevance. With respect to BtC values, the most relevant authors are Robin D. Rogers and Richard P. Swatloski, both highly representative for big specialty B – Ionic Liquids, indicating their contribution to promote interaction between these two research topics.

Atsushi Takagaki, Michikazu Hara, David M. Alonso and James Dumesic can be considered the intellectual hubs of the big specialty C – Biomass, due to their high coverage and their number of papers on the research fronts, indicating their high contribution to set work themes and spread research on biomass. Other important authors are Joseph J. Bozell and Gene R. Peterson, whose work has high circulation among the scientific community. James A. Dumesic has a very important role as intellectual authority in this specialty, as he is the author who publishes the most, and whose texts have aroused the interest of the scientific community (high CB and CF). Other authors who also play an important role as intellectual authorities are George W. Huber, Avelino Corma and Sara Iborra.

D – Catalysis. This big specialty has the second largest research front, with 46 papers published between 1999 and 2014. Michikazu Hara has the highest coverage and is also high-ranking in number of appearances on the research front (LCS) (Table 8). Xuezheng Liang, Chenze Qi and Daizo Yamaguchi follow Hara on coverage ranking, but have low

Table 7. Big specialty C – Biomass, most relevant authors of the intellectual base.

Authors	NP C	Total NP	N BSp	CB C	Total CB	BtC C	Total BtC	CF C	Total CF
DUMESIC, JA	9	9	1	113.47	113.47	0.04	0.04	661	661
HUBER, GW	5	5	1	66.23	66.23	0.01	0.01	556	556
KOBAYASHI, S	4	5	2	8.58	16.72	0.1	0.1	22	73
ALONSO, DM	4	4	1	60.87	60.87	0.04	0.04	221	221
CHHEDA, JN	4	4	1	39.5	39.5	0	0	333	333
CORMA, A	3	5	2	67.29	92.1	0.08	0.08	717	772
HACHIYA, I	3	3	1	3.96	3.96	0.04	0.04	15	15
IBORRA, S	3	3	1	67.29	67.29	0.08	0.08	717	717
ROMAN-LESHKOV, Y	3	3	1	30.25	30.25	0	0	219	219
ROGERS, RD	2	12	3	17.97	149.52	0.15	0.27	218	612
SWATLOSKI, RP	2	9	2	17.97	94.37	0.15	0.22	218	359
BOND, JQ	2	2	1	39.97	39.97	0.04	0.04	155	155
GALLEZOT, P	2	2	1	62.15	62.15	0	0	179	179
DAVISON, BH	2	2	1	36.25	36.25	0.15	0.15	241	241
RAGAUSKAS, AJ	2	2	1	36.25	36.25	0.15	0.15	241	241
TSCHAPLINSKI, T	2	2	1	36.25	36.25	0.15	0.15	241	241
HOLBREY, JD	1	8	2	6.96	114.85	0.14	0.21	197	403
SPEAR, SK	1	2	2	6.96	25.08	0.14	0.14	197	256
VELTY, A	1	1	1	19.77	19.77	0.07	0.07	381	381
BRITOVSEK, G	1	1	1	6.42	6.42	0.13	0.13	165	165
CAIRNEY, J	1	1	1	6.42	6.42	0.13	0.13	165	165

GCS, indicating that their work does not have much circulation within the academic community. Rajender S. Varma is a prominent author within this specialty, having the highest number of citations, the highest number of papers and high coverage.

The intellectual base of this big specialty consists of 61 papers, published between 1981 and 2017. Rajender S. Varma, Roger Sheldon, Paul T. Anastas and André Loupy are the most recurring authors (Table 9). Sheldon has a large number of papers in this intellectual base, but also in other major specialties, showing that his research is not as specialized, whereas Anastas has 6 appearances (out of 9) in big specialty D – Catalysis, highest CB value, as well as the largest highest number of accumulated citations and BtC, showing his expertise in this field. Tracy C. Williamson, Mary M. Kirchhoff and Nicolas Eghbali are co-authors with Anastas; they appear among high-ranking authors in CF, CB and BtC. Varma's influence is corroborated by his high CF, CB and BtC

Table 8. Big specialty D – Catalysis, most relevant authors of the research front.

Author	Cov D	Total Cov	GCS D	Total GCS	LCS D	Total LCS	N BSp
HARA, M	0.279	0.0707	194	485	3	7	2
LIANG, XZ	0.264	0.0438	22	22	3	3	1
QI, CZ	0.264	0.0438	22	22	3	3	1
YAMAGUCHI, D	0.197	0.0381	63	126	2	4	2
VARMA, RS	0.181	0.0434	2060	3938	4	6	3
HAYASHI, S	0.179	0.0486	89	249	2	4	2
GUO, Y	0.130	0.0216	134	134	2	2	1
KATO, H	0.114	0.0217	63	126	1	2	2
KITANO, M	0.114	0.0217	63	126	1	2	2
NAKAJIMA, K	0.114	0.0217	63	126	1	2	2
SUGANUMA, S	0.114	0.0217	63	126	1	2	2
GUO, YX	0.098	0.0163	14	14	1	1	1
XIAO, HQ	0.098	0.0163	14	14	1	1	1
HU, BW	0.083	0.0137	2	2	1	1	1
LI, CQ	0.083	0.0137	2	2	1	1	1

values. Loupy and Polshettiwar also have high CB, indicating that they have developed research that has leveraged investigations into this major specialty at certain periods.

In analyzing the authors of the research front, Rajender S. Varma and Michikazu Hara may be considered to be the most important intellectual hubs, largely responsible for promoting the cohesion of this big specialty around common research topics. Varma is also a strong intellectual authority, as he has a large number of papers, and high CF and CB. Other important authors are André Loupy and Vivek Polshettiwar, with large numbers of papers, and high CB and accumulated CF. Paul T. Anastas is greatly influential in the specialty, despite his output consisting of more general papers on GC.

E – GC Characterization. This specialty is formed by a single large cluster that has the largest research front (even when compared to the big specialties), with 56 published papers between 1999 and 2017. This specialty is plural in its themes, grouping papers concerned with laying the foundations, challenges and possibilities of GC, as well as setting its themes. The authors with the highest accumulated coverage are Paul T. Anastas, Roger A. Sheldon and James H. Clark, all of whom are highly known in the field, which can be seen by the high number of citations they receive (Table 10).

With regard to the intellectual base, it contains 45 works (the 5th largest if compared to the big specialties), published between 1991 and 2016. Roger A. Sheldon is the author with the highest number of works in the intellectual base of this specialty, although a large number of his papers is to be found in other specialties, thus showing he has more transversal influence throughout GC (Table 11). James H. Clark, David J. C. Constable, Alan D. Curzons and Barry M. Trost have a large number of papers with great focus on

Table 9. Big specialty D – Catalysis, most relevant authors of the intellectual base.

Authors	NP D	Total NP	N BSp	CB D	Total CB	BtC D	Total BtC	CF D	Total CF
VARMA, RS	7	9	2	86.48	118.59	0.16	0.21	341	426
SHELDON, R	6	23	5	26.64	275.84	0.02	0.5	221	1718
ANASTAS, P	6	9	2	85.36	115.73	0.28	0.46	1065	2410
LOUPY, A	5	5	1	70.51	70.51	0.02	0.02	148	148
POLSHETTIWAR, V	3	4	2	55.41	66.15	0.03	0.03	180	199
DOMEN, K	3	3	1	46.33	46.33	0.09	0.09	139	139
HARA, M	3	3	1	46.33	46.33	0.09	0.09	139	139
HAYASHI, S	3	3	1	46.33	46.33	0.09	0.09	139	139
KONDO, JN	3	3	1	46.33	46.33	0.09	0.09	139	139
ARENDS, I	3	3	1	15.54	15.54	0.01	0.01	180	180
WILLIAMSON, TC	2	3	2	35.93	50.41	0.09	0.27	116	1229
PETIT, A	2	2	1	32.71	32.71	0	0	57	57
TANAKA, K	2	2	1	19.82	19.82	0.1	0.1	268	268
KIRCHHOFF, MM	2	2	1	18.53	18.53	0.15	0.15	532	532
POLIAKOFF, M	1	6	5	0	41.82	0	0.02	182	354
METZGER, JO	1	3	2	8.15	19.88	0.11	0.13	14	33
TODA, F	1	2	2	0	0	0.08	0.11	220	225
EGHBALI, N	1	1	1	32.89	32.89	0.07	0.07	238	238
FARREN, TR	1	1	1	0	0	0	0	182	182
FITZPATRICK, JM	1	1	1	0	0	0	0	182	182

this specialty. These authors also have high CF, CB and BtC values, corroborating their strong role in substantiating the characterization of GC. Concepción Jiménez-González has a high CB value, showing that her ideas have aroused great interest. Philip G. Jessop accumulates great BtC value, indicating his role in promoting interaction between this specialty and the others. Average CB of this specialty spanned from 2007 to 2011.

As pointed above, most outstanding authors on the research front in this specialty are Paul T. Anastas, Roger A. Sheldon and James H. Clark, indicating that they are intellectual hubs, responsible for bringing together the discussion about what GC is and how to evaluate it, as well as in spreading the principles and procedures of this field. The intellectual base of this specialty shows us that Sheldon and Clark are also important intellectual authorities, developing research that provides important information for GC characterization. David J. C. Constable, Alan D. Curzons and Barry M. Trost also play an important role as intellectual authorities in the characterization of GC. We shall later

Table 10. Specialty E – GC Characterization, most relevant authors of the research front.

Author	Cov E	Total Cov	GCS E	Total GCS	LCS E	Total LSC	N BSp
ANASTAS, P	0.19	0.071	1561	5198	3	9	5
SHELDON, RA	0.13	0.049	433	1402	2	4	3
CLARK, JH	0.13	0.016	625	625	1	1	1
LAWRENSON, S	0.11	0.013	18	18	2	2	1
NORTH, M	0.11	0.022	18	595	2	3	2
VACCARO, L	0.11	0.013	56	56	2	2	1
NAMIESNIK, J	0.11	0.022	93	180	2	3	2
PENA-PEREIRA, F	0.11	0.022	93	180	2	3	2
EGHBALI, N	0.11	0.039	891	4455	1	5	5
JEROME, F	0.09	0.027	279	575	2	4	3
ACKERMANN, L	0.09	0.011	16	16	1	1	1
BAO, WL	0.09	0.011	10	10	1	1	1
BOUSFIELD, TW	0.09	0.011	4	4	1	1	1
BUCO, A	0.09	0.011	1	1	1	1	1
CAMP, JE	0.09	0.011	4	4	1	1	1

discuss the existence of hubs and intellectual authorities for the whole field of GC, extrapolating the limits of specialist expertise.

F – CO_2 as substrate. Specialty F – CO_2 as Substrate has the smallest research front (18 works) and the smallest intellectual base (28); although it is thematically close to C – Biomass, it presents a co-citation network with very distinct characteristics, forming an isolated specialty. In their research front, Johannes Steinbauer and Thomas Werner are notable for their high coverage (0.47 each) and number of papers (4 each), which are co-authored by Hendrik Büttner, Lars Longwitz and Christoph Wulf (Table 12).

Within the intellectual base of the specialty F – CO2 as Substrate, we can highlight the contributions of Toshiyasu Sakakura and his co-author, Jun-Chul Choi, with a high number of papers, CF and accumulated BtC (Table 13). Philip G. Jessop and Walter Leitner published papers in collaboration, and also have high number of publications, highest accumulated CB and BtC in this specialty. Average CB spanned from 2005 to 2008, a very early topic of interest.

The above shows that Johannes Steinbauer and Thomas Werner are intellectual hubs of the specialty F – CO_2 as Substrate, due to their high coverage and number of papers on the research front. Intellectual authorities of this specialty may be Toshiyasu Sakakura, Jun-Chul Choi, Philip G. Jessop and Walter Leitner, for the number of papers, CF and accumulated CB values on the intellectual base.

Table 11. Specialty E – GC Characterization, most relevant authors of the intellectual base.

Authors	NP E	Total NP	N BSp	CB E	Total CB	BtC E	Total BtC	CF E	Total CF
SHELDON, R	9	23	5	108.85	275,84	0.38	0,5	1053	1718
CLARK, J	6	8	3	14.52	48.86	0,05	0,05	253	384
TROST, BM	4	4	1	32.55	32.55	0.3	0.3	737	737
CONSTABLE, DJC	4	4	1	27.43	27.43	0,12	0,12	475	475
CURZONS, AD	4	4	1	27.43	27.43	0,12	0,12	475	475
ANASTAS, P	3	9	2	30.37	115.73	0,18	0.46	1345	2410
DUNN, PJ	3	3	1	30.23	30.23	0,05	0,05	303	303
PRAT, D	3	3	1	0	0	0.04	0.04	59	59
HORVATH, IT	2	6	3	18.72	77.42	0	0,03	170	306
MACQUARRIE, DJ	2	3	2	10.56	19.87	0	0	16	32
JIMENEZ-GONZALEZ, C	2	2	1	45.59	45.59	0.08	0.08	222	222
CUNNINGHAM, VL	2	2	1	0	0	0,1	0,1	316	316
JESSOP, PG	1	6	4	21.26	89,5	0,15	0,32	123	279
WILLIAMSON, TC	1	3	2	14.48	50.41	0,18	0,27	1113	1229
JEROME, F	1	3	3	19.42	63,23	0,13	0.2	60	180
GU, YL	1	2	2	19.42	35.02	0,13	0.19	60	93
BROXTERMAN, QB	1	1	1	23	23	0,06	0,06	71	71
MANLEY, JB	1	1	1	23	23	0,06	0,06	71	71
PONDER, CS	1	1	1	23	23	0,06	0,06	71	71

4.2 Results Validation

In 2016, the *Green Chemistry Journal* published a series of 13 editorials commemorating the 25 years of GC, penned by renowned authors of the field, showcasing the advances made in each of the Twelve Principles. By crossing the authors of these editorials and their references with the results of this research, it is possible to provide indications of the relevance of the results found. Two out of the 14 different intellectual hubs wrote papers for the commemorative editorials, and two are listed in their references, so that 29% of the hubs are related to these editorials. Anastas, an important GC hub, writes with Han, Leitner and Poliakoff [2] the opening editorial of the commemorative series, and also appears as a reference in almost all editorials, being related to all principles except 12 – Inherently Safer Chemistry [25]. Sheldon (GC hub and authority) is the author of the editorial on Principle 2 – Atom economy [18], and appears as a reference in six editorials [19–24]. Hara (hub of big specialties C – Biomass and D – Catalysis) appears in the editorial references of Delidovich and Palkovits [19] on Principle 9 – Catalysis. On the other hand, Clark (hub and authority of specialty E – GC Characterization), appears on

Table 12. Specialty F – CO_2 as substrate, most relevant authors of the research front.

Author	Cov F	Total Cov	GCS F	Total GCS	LCS F	Total LCS	N BSp
STEINBAUER, J	0.47	0.0432	34	53	4	7	2
WERNER, T	0.47	0.0432	34	53	4	7	2
BUTTNER, H	0.25	0.0215	23	31	2	3	2
LONGWITZ, L	0.25	0.0240	10	20	2	4	2
WULF, C	0.25	0.0215	23	31	2	3	2
CANELLAS, S	0.14	0.0107	1	1	1	1	1
JOSE, T	0.14	0.0107	1	1	1	1	1
KLEIJ, AW	0.14	0.0107	1	1	1	1	1
PERICAS, MA	0.14	0.0107	1	1	1	1	1
GARCIA, H	0.11	0.0084	102	102	2	2	1
CAO, CY	0.11	0.0084	3	3	1	1	1
CHOI, JC	0.11	0.0084	1	1	1	1	1
DINDAROGLU, M	0.11	0.0084	15	15	1	1	1
FUKAYA, N	0.11	0.0084	1	1	1	1	1
Gao, XT	0.11	0.0084	2	2	1	1	1

the editorials on Principles 2 – Atom Economy [18], 9 – Catalysis [19] and 8 – Reduce Derivatives [20].

There are 21 different intellectual authorities, twelve of which are related to the editorials (57%). Chao-Jun Li is an authority of big specialty A – Solvents, and author of the editorial on Principle 8 – Reduce Derivatives. Corma and Iborra (authorities of C – Biomass) feature in the references to the editorial on Principles 9 – Catalysis [19] and 7 – Use of Renewable Feedstocks [21]. Constable and Curzons (authorities of E – GC Characterization) are featured in the references to the editorials on Principles 8 – Reduce Derivatives [20], 6 – Design for Energy Efficiency [22], and 12 – Inherently Safer Chemistry [25]. Trost, also authority in E – GC Characterization, appears in the references to the editorials on Principles 8 – Reduce Derivatives [20] and 2 – Atom Economy [18]. Jessop is an important intellectual authority in F – CO_2 as Substrate, and appears as author to the editorial on Principles 5 – Safer Solvents and Auxiliaries [26] and as a reference in 8 – Reduce Derivatives [20]. Leitner, also authority in F – CO_2 as Substrate, is present in the references to the editorials on Principles 3 – Less Hazardous Chemical Synthesis [24], 6 – Design for energy efficiency [22] and 8 – Reduce Derivatives [20]; he is also author of the opening editorial [2] Toshiyasu Sakakura and Jun-Chul Choi, both authorities in F – CO_2 as Substrate, are references in editorial about 3 – Less Hazardous Chemical Synthesis [24].

We may also note that many of the intellectual hubs are not mentioned in the commemorative editorials. This may be due to the fact that they are authors more closely

Table 13. Specialty F – CO_2 as Substrate, most relevant authors of the intellectual base.

Authors	NP F	Total NP	N BSp	CB F	Total CB	BtC F	Total BtC	CF F	Total CF
SAKAKURA, T	3	3	1	25.05	25.05	0.04	0.04	229	229
JESSOP, PG	2	6	4	44.1	89.5	0.07	0.32	116	279
LEITNER, W	2	4	3	39.04	48.93	0.09	0.1	118	134
CHOI, JC	2	2	1	12.18	12.18	0.04	0.04	167	167
ROGERS, RD	1	12	3	18.12	149.52	0	0.27	59	612
CLARK, J	1	8	3	9.31	48.86	0	0.05	16	384
POLIAKOFF, M	1	6	5	7.57	41.82	0	0.02	13	354
BECKMAN, EJ	1	4	3	18.17	36.39	0	0.02	44	87
IKARIYA, T	1	3	2	21.16	33.2	0.04	0.13	37	57
NOYORI, R	1	3	2	21.16	33.2	0.04	0.13	37	57
HUDDLESTON, JG	1	3	2	18.12	73.34	0	0.11	59	201
YOSHIDA, T	1	3	2	5.05	27.46	0	0	8	72
TUNDO, P	1	2	2	20.02	30.42	0	0	64	154
KOHNO, K	1	1	1	12.87	12.87	0	0	62	62
YASUDA, H	1	1	1	7.34	7.34	0.04	0.04	159	159
SELVA, M	1	1	1	20.02	20.02	0	0	64	64
SHAIKH, AAG	1	1	1	12.04	12.04	0.03	0.03	65	65
SIVARAM, S	1	1	1	12.04	12.04	0.03	0.03	65	65
BORNER, A	1	1	1	0	0	0.05	0.05	17	17
SCHAFFNER, B	1	1	1	0	0	0.05	0.05	17	17
SCHAFFNER, F	1	1	1	0	0	0.05	0.05	17	17
VEREVKIN, SP	1	1	1	0	0	0.05	0.05	17	17

connected with recent and transient literature, while editorials were focused on presenting the advancements and milestones in GC – which corroborates the fact that almost 60% of intellectual authorities are related to the editorials. It should also be taken into account that editorials are structured around principles, not specialties or research themes, which may explain why none of the hubs or intellectual authorities of big specialty B - Ionic Liquids are related to the editorials, as well as account for the great participation of author of specialty E – GC Characterization.

5 Final Remarks

Table 14 presents a summary of the most important authors in each specialty. Authors in the research fronts from each specialty were assessed by the accumulated coverage

of their output, generating the roll of 14 researchers that act as intellectual hubs of GC specialties. As the research front is about the most relevant and fresh research in certain time, these intellectual hubs are the major responsible for divulgating, sharing and organizing an specialty around an research object. The knowledge in the research fronts are built upon the previous selected knowledge, described in the intellectual base, from where authors with high significance functions as intellectual authorities to their specialties. Twenty-one researchers contribute with fundamental knowledge to sustain certain GC specialties. Surely, those names (either hubs or authorities) are not the only ones structuring the GC field, neither they are responsible for all the knowledge in this research branch. But they have special significance in funding and spreading the GC practices.

Table 14. GC hubs and intellectual authorities and their specialties.

Specialties	Hubs	Authorities
A – Solvents	Victorio Cadierno Javier Francos	Chao-Jun Li
B – Ionic Liquids	Robin D. Rogers Kenneth R. Seddon	Kenneth R. Seddon Robin D. Rogers Tom Welton Peter Wasserscheid
C – Biomass	David M. Alonso James A. Dumesic Atsushi Takagaki Michikazu Hara	James A. Dumesic George W. Huber Avelino Corma Sara Iborra
D – Catalysis	Rajender S. Varma Michikazu Hara	Rajender S. Varma André Loupy Vivek Polshettiwar
E – GC Characterization	Paul T. Anastas Roger A. Sheldon James H. Clark	Roger A. Sheldon James H. Clark David J. C. Constable Alan D. Curzons Barry M. Trost
F – CO_2 as substrate	Johannes Steinbauer Thomas Werner	Philip G. Jessop Walter Leitner Toshiyasu Sakakura Jun-Chul Choi

This research allows for a better understanding of the structure of GC and can assist researchers in searching for relevant information about topics of interest. Co-citation analysis was a suitable strategy for the analysis of groupings, and the use of its metrics showed to be relevant for determining hubs and intellectual authorities in the field. However, the lack of author keywords in some journal, such as Green Chemistry, proved to hurdle the information retrieval. Also, the changing of algorithm for Keywords Plus in

Web of Science makes it difficult to retrieve the same registers nowadays. A thoughtful standardization of databases and indexation is required and is a fact worth taking into account in future research. Comparisons with qualitative descriptions made in the field corroborate the coherence of the results of this research, and eventual discrepancies seem to reflect differences in the approach to information in the field: the analyses made by experts start from the Twelve Principles as prior categories for the organization of the GC, while this research draws specialties from the field's own citation patterns. This seems to be a more coherent strategy with the current GC target of thinking the Twelve Principles in a comprehensive, interdependent way, overcoming the incremental vision based on isolated principles [8].

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