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Abstract

In the late 1990s chemists were among the early adopters of open access (OA) publishing. As it happened with preprints, the early successful adoption of OA publishing from chemists subsequently slowed down. In 2016 chemistry was found to be the discipline with the lowest fraction of OA papers amid papers in all fields published between 2009 and 2015. To benefit from open science in terms of enhanced citations, collaboration, job and funding opportunities, chemistry scholars need updated information (and education) on open science of practical relevance. Suggesting avenues for quick uptake of OA publishing from chemists in both developed and developing countries, this study offers a critical perspective on academic publishing in the chemical sciences that will be useful to inform the aforementioned education.

1 Introduction

Chemistry scholars in the late 1990s were amid the early adopters of open access (OA) publishing in the digital era, namely of publishing scientific articles and reviews in journals freely accessible on the internet. Writing in 2007 in one such new OA journal, Hodd reported that in chemistry there were "currently over 50 open access journals" [1]. Examples include *Arkivoc* publishing OA papers in synthetic organic chemistry since 2000, and the *Beilstein Journal of Organic Chemistry* launched in 2005. Both journals do not require authors to pay an article processing charge (APC).

Publishing scientific articles accessible without restrictions largely improves the visibility of the freely accessible study. Accordingly, comparing the number of citations of articles in physics published between 1992 and 2002 made OA by self-archiving with the citations of articles from the *same* journals that were not made OA by their authors, in 2004 Harnad and Brody first unveiled that the OA/non-OA citation ratio varied between 2.5 and 5.7 [2].

As it happened with preprints [3], the early successful adoption of OA publishing amongst chemistry scholars subsequently faded away. As a result, with less than 20% papers being freely available in 2016 chemistry was found to be the discipline with the lowest fraction of OA papers amid 100,000 research papers published between 2009 and 2015 [4]. For comparison, the same statistical analysis found that more than 50% of biomedical research and mathematics papers were freely accessible.

The advantages in terms of enhanced visibility, number of citations, career and funding opportunities of open science, however, are too numerous for chemistry scholars continuing to ignore open science. In 2018, the percentage of chemistry papers published as open access (in the Web of Science category "chemistry multidisciplinary") increased to 26% of the total [5].

Showing evidence of enhanced impact of OA journals, in 2017 the top three most cited multidisciplinary scientific journals were all fully OA journals (Table 1).

Table 1 . Top five multidisciplinary scientific journals ranked by number of citations in 2017. [Source: Clarivate Analytics, 2018].

Rank	Journal	Number of citations
1	*PLOS One*	138,828
2	*Scientific Reports*	128,437
3	*Nature Communications*	83,086
4	*Nature*	73,840
5	*Science*	67,088

Alone, as remarked by Markram [6], the number of citations of*PLOS One* (138,828) in 2017 was only slightly lower than the number of citations of *Science* and *Nature* combined (140,928), whereas the number of the top citations of the top three journals (350,351) was more than twice as large as that of the latter subscription journals combined.

Under these circumstances, continuing to rely on the old publication model for which manuscripts are sent for peer review waiting 9 months (for chemistry articles published in 2013 [7]), is no longer tenable also in chemistry.

Likewise to many other scholars, most research chemists have never received formal education on publishing scientific articles in the digital age [8]. Hence, what chemistry scholars currently need is updated information (and education) on open science of practical relevance to their work. It is enough to conduct a Boolean search on Google Scholar using the queries "open access" and "chemistry" or "open science" and "chemistry" to find out that few studies have been devoted to the role of open science in chemistry [1,9,10,11], including three studies [3, 12,13] on preprints in chemistry.

Suggesting avenues for quick uptake of OA publishing from research chemists in both developed and developing countries, this study offers a critical perspective on academic publishing in the chemical sciences that will be useful to inform the aforementioned education.

2 Current state of open access publishing in chemistry

By early November 2020, for the subject "chemistry" the Directory of Open Access Journals listed 144 OA journals, 72 of which did not levy any APC [14]. Table 2 lists selected titles and fields amid the latter journals.

Table 2 . Ten selected OA chemistry journals not levying an APC.

Field	Journal
Organic chemistry	*Arkivoc*
Organic chemistry	*Beilstein Journal of Organic Chemistry*
Materials chemistry	*Beilstein Journal of Nanotechnology*
All fields	*Chemical Science*
All fields	*ACS Central Science*
Lipid science	*Grasas y Aceites*
All fields	*CHIMIA*
History of chemistry	*Substantia*
Materials chemistry	*Nanochemistry Research*
Surfaces and interfacial phenomena	*Journal of Applied Surfaces and Interfaces*

An increasing number of national chemistry societies publish OA journals devoid of publishing costs for authors and their employers. The Swiss Chemical Society, for example, publishes *CHIMIA* both digitally at the URL http://chimia.ch/ and in print. Listed (indexed) in the most important databases for chemistry research, the journal is published 10 times a year and in 2019 had a journal impact factor (JIF) of 1.478.

Similarly, the Iranian Chemical Society publishes *Nanochemistry Research* . In 2015 the ACS launched *ACS Central Science* which, like *Chemical Science* published by the Royal Society of Chemistry, does not levy any APC. For comparison, the latter journal in 2019 published 1,306 articles, while in the same year *ACS Central Science* published 247 studies.

Public research bodies too publish OA chemistry journals such as in the case of *Grasas y Aceites* published by Spain's Research Council (CSIC) Instituto de la Grasa. Published on the CSIC website at http://revistas.csic.es/ in one yearly volume, divided into four quarterly issues appearing in March, June, September and December, the journal (JIF 1.440 in 2019), is a key literature reference for all scholars working in the field of lipid science and technology.

Similarly since 2017, the University of Florence publishes on the website of Firenze University Press at https://riviste.fupress.net/index.php/subs the journal *Substantia* . Though focusing on the history of chemistry the journal publishes also special issues with studies from eminent scholars that go from "Open science" [15] through "Water in biology: what's so special about it?" [16].

Large chemistry publishers publish several OA chemistry journals (Table 3) generally adopting the APC as a source of revenues.

Table 3 . Ten selected OA chemistry journals levying an APC.

Field	Journal
All fields	*ChemistryOpen*
All fields	*JACS Au*
All fields	*RSC Advances*
All fields	*ACS Omega*
All fields	*BMC Chemistry*
Polymer science	*Polymers*
All fields	*Open Chemistry*
Catalysis science	*Catalysis, Structure & Reactivity*
Green chemistry	*Current Research in Green and Sustainable Chemistry*
Organic chemistry	*PeerJ Organic Chemistry*

In 2008 Springer acquired BioMed Central Group, an OA publisher founded in Great Britain in 2000 publishing at the time of the acquisition some 180 journals including 7 chemistry journals [17]. Wiley started to publish *ChemistryOpen* in 2012 in partnership with the ChemPubSoc Europe, a consortium of 16 continental European chemical societies [5].

In 2015 the Royal Society of Chemistry converted its journal *Chemical Science* to an OA journal and waived the APC. The subsequent year, the same publisher converted *RSC Advances* (the world's largest chemistry subscription journal with 13,287 published articles published in 2016) to open access setting the APC at £500 for all authors for the first two years (2017 and 2018), and then at £750.

Due to introduction of the APC, the publisher expected the journal to publish "in the region of 7,000 articles in 2017" [18], remaining the largest chemical science journal. Indeed, in 2017 the journal published 6,675 articles, followed by 4,767 paper in 2018 and 4,801 in 2019 [19].

Chemistry scholars willing to publish their studies in open access can opt also for publication in multidisciplinary OA journals, many of which are owned by well-established publishers. Examples include *Scientific Reports* and *Nature Communications* (Springer), *Science Advances* (American Association for the Advancement of Science), *Advanced Science* (Wiley), and *Heliyon* (Elsevier). Owned by a nonprofit publisher, *PLOS One* is another cross-disciplinary OA journal publishing also chemistry studies.

Finally, most publishers of chemistry journals allow to make individual articles open access upon payment of an APC. The resulting journals allowing this option are called "hybrid" journals to distinguish them from fully open access journals. "Gold" and "platinum" open access journals indicate, respectively, journals for which the publisher levies or does not levy an APC. Originally, the color codes to classify journals included "gold" providing immediate OA to research articles, and "green" allowing authors to deposit their peer-reviewed manuscripts in OA repositories after an embargo period [20].

Table 4 . APC values in different currencies for selected chemistry and multidisciplinary journals as of late 2020.

Journal	**Article processing charge**
ChemistryOpen	EUR 1,800
JACS Au	USD 5,000*
RSC Advances	GBP 750
ACS Omega	USD 1,250
BMC Chemistry	GBP 1,570
Polymers	CHF 1800
Open Chemistry	EUR 1,200
Current Research in Green and Sustainable Chemistry	USD 2250
PLOS One	USD 1,695
Science Advances	USD 4,500
Advanced Science	USD 5,000
Nature Communications	GBP 3,790
Heliyon	USD 1,750

*Selecting CC-BY license, USD 4,000 when selecting CC-BY-NC-ND license.

In chemistry too the APCs present significant differences across different OA journals (Table 4). As lately shown by economics scholars, this large variance is not explained by the cost of production but by other drivers collectively identified by the scholars as "market power" [21].

In detail, the average APC can be modeled a constant term of \$768.1, interpreted as the production cost of processing an article for an OA journal, plus the JIF×132.5 (a one unit increase of the JIF increases the APC by \$132.5), plus the compound effect of being a big publisher amounting to \$447.6 + \$1.13 × pub age. big. pub, namely the product of publisher age and size because age only counts in combination with being a big publisher (otherwise age increases average APC by only \$1.13) [21].

3 The structure of the chemistry publishing industry

Trying to answer the question why in 2017 scholars continued "to give their labour – as authors, referees and editors – to publishing firms that do not, in fact, circulate knowledge widely and affordably" [22], a team of scholars in open science suggests that:

> ≪The answer lies in a lack of detailed understanding among academics of the historical and economic forces at play in academic publishing; and in the success with which big publishers have learned how to make themselves apparently indispensable to the academic prestige economy≫ [22].

Data in Table 5 show the average citations per paper over a 3-year window (2017-2019) for the 20 largest publishers by volume (total documents in 2019) [23].

Table 5 . Top 20 publishers by volume, ranked by number of average citations received to articles published in 2016, 2017 and 2018. [Source: SCImago, 2019].

Rank	**Publisher**	**Average citation**
1	American Chemical Society	6.88
2	Royal Society of Chemistry	5.13
3	American Physical Society	4.29
4	Oxford University Press	3.82
5	Frontiers	3.63
6	Elsevier	3.59
7	MDPI	3.3
8	PLOS	3.3
9	Wiley	3.27
10	IEEE	2.75
11	Springer Nature	2.63
12	Institute of Physics	2.1
13	SAGE	2
14	Wolters Kluwer	1.97
15	Hindawi	1.94
16	American Institute of Physics	1.7
17	Taylor & Francis	1.59
18	Cambridge University Press	1.54
19	Walter de Gruyter	1.16
20	Science Press	1.01

The American Chemical Society and the Royal Society of Chemistry, each publishing tens of subscription journals, lead the ranking. Furthermore, referring to articles published by the aforementioned learned societies over the previous 3-year window (2015-2017), the average number of citations per paper was substantially *higher* for subscription journals when compared to OA journals [6].

Alone, these two facts help to explain why in 2018 still 74% of the chemistry papers were published in subscription journals [5]. Chemistry is the most concentrated segment of the scientific publishing industry, with only five publishers publishing more than 70% of chemistry studies in 2013 [24]. More recently, with 207 journals from 20 publishers, chemistry was found to be the third (after multidisciplinary and space science) scientific discipline in terms of market concentration measured by the Herfindahl-Hirschman index [21].

Another highly reputed learned society, the American Physical Society, ranks third amid the largest 20 publishers classified by number of average citations received to articles published in 2016, 2017 and 2018 displayed in Table 5. In this case, however, the number of citations of articles published in OA journals is almost *twice* higher than that in non-OA journals [6]. The reason is due to the fact that physicists are familiar with OA papers thanks both to preprints posted in arXiv since the early 1990s and widespread use of "green" self-archiving.

4 Openly accessible, impactful science

"If you include journal impact factors in the list of publications in your curriculum", wrote Curry citing the Seglen's 1992 work [25] showing the highly skewed pattern of citation distribution for which only a few papers in a journal account for most of the journal's total citations, "you are statistically illiterate" [26].

Now, given the fact that universities and research bodies continue to use the journal impact factor and other citation-based metrics such as the h-index [27] to evaluate researchers and for granting research funds, it is not surprising that researchers continue to strive to publish in high JIF journals.

For example, in a few months some 34,000 biologists signed the online petition initiative by Varmus, Brown, and Eisen calling by late 2000 all scientists to "pledge that, beginning in September 2001, we will publish in, edit or review for, and personally subscribe to only those scholarly and scientific journals that have agreed to grant unrestricted free distribution rights to any and all original research reports that they have published, through PubMed Central and similar online public resources, within 6 months of their initial publication date" [28]. Actually, most signatories continued to publish their work in paywalled journals (and to review journal manuscripts for free, as well).

Yet, as noted by Harnad in 2005 [29], over 90% of journals gave author the permission to self-archive their papers on personal websites or in institutional repositories. Underlining the inconsistency, Harnad continued:

> ≪Now SUPPOSE that – in addition to performing the keystrokes required to sign the 2001 *PLOS* open letter (pledging to boycott journals unless they become OA journals), each of the 34,000 *PLOS* signatories had also performed (or deputized a librarian, secretary or student to perform for them) the few further keystrokes it would have required to make just one of their own year-2001 articles OA by self-archiving it, free for all, on the web. ≪THEN the number of OA articles (34,000) resulting from just that minimal act would already have doubled (to 60%) the percentage of OA articles (34%) among the approximately 55,000 Biology articles indexed by ISI in 2001; it would also have exceeded the total number of articles published by both BioMed Central and *PLOS* journals from 2001 to the present (c. 20,000) [29]≫

The very same inconsistency was noted in 2014 for scholars of all disciplines upon analyzing 1,066,079 articles published between 1999 and 2011 (social sciences 91,729 articles, life sciences 202,833 articles, health sciences 282,096 articles, and physical sciences 489,421 articles), 80.4% of which could be self-archived after one year of publication either on personal webpages (78.1 % of articles) or in institutional repositories (79.9%), whereas around 12% of total annual articles are actually self-archived [30].

"The results" wrote Laakso concluding the study, "highlight the substantial unused potential for green OA" [30]. This fact provides evidence that today's scholars in large part are unaware of the possibilities offered by today's scholarly communication and further substantiates my viewpoint for which the full transition to open science requires new education of today's doctoral students and early career researchers on scholarly communication in the digital era [8].

5 Outlook and Conclusions

OA academic publishing is thriving. In 2019, MDPI, an OA multidisciplinary publisher jointly established by a former research chemist in 1996, became the 5$^{\text{th}}$ world's largest academic publisher with over 106,000 articles published in one year only [31]. Several MDPI journals are devoted to chemistry, nanotechnology and materials science. The APCs across the aforementioned journals are in the order of CHF 1,600. Most publishers of "gold" OA journals offer discounts on the APCs, for example to scholars submitting from developing countries, and even waive them in certain cases.

Given the APC levels shown in Table 4 it may not be surprising to learn that even in the USA, a wealthy nation leading for over a century the global scientific production, OA publishing in journals levying an APC is used in a disproportionately larger fraction from professors at elite institutions [32], namely at research centres receiving huge grants.

With the early success of the Chemistry Preprint Server (CPS) publishing some 500 studies from scholars based in 51 countries two years after its launch in August 2000 http://preprint.chemweb.com [33], research chemists were the first after physicists, mathematicians and computer scientists to show real interest in open science. Today, the fact that chemistry scholars understand and value open science is shown for example by PubChem, an online repository for information on chemical substances and their biological activities, that 11 years after its inception in 2004 already hosted at https://pubchem.ncbi.nlm.nih.gov more than 157 million chemical substance descriptions [34].

Put simply, most research chemists never received education on today's scholarly communication and on open science. The result is that still in the early 2020s, the vast majority of them does not self-archive research papers in institutional and personal websites, thereby losing the opportunities for enhanced *use* (and citation) of their own work.

Whether new chemical methods, materials, ideas or models, the main objective of any chemistry scholar is to see her/his findings *used* by the global chemistry community which, unique amid all scientific disciplines, includes researchers working for a huge global industry comprising chemical (and pharmaceutical) companies which is central to the wealth of any country [35].

Likewise to any other scholar in the basic sciences, chemistry scholars are also interested in citations which still place a central role in review, promotion and tenure procedures used by their employers. By quickly fulfilling the "unused potential for green OA" [30], chemistry scholars should make their papers openly accessible through self-archiving on institutional or personal websites, and publish in preprint form any new works. Beyond recording rapid increase in the number of citations, the same scholars will enjoy the benefits of open science in terms of enhanced collaboration, job and funding opportunities [36,37].

In other words, rather than paying the APCs of "gold" OA journals, chemistry scholars should take advantage of the new tools enabled by the internet and by progress in scholarly communication, freely publishing their own work first as preprint and then in any journal not levying any APC, namely "platinum" OA journals or even in "paywalled" journals. After the embargo period (often 12 months, but for certain journals 24 months), the published article will be self-archived either in institutional or personal websites.

In promotion and tenure processes, chemistry scholars are chiefly evaluated based on research, with evaluation often failing to reward teaching and service devaluing faculty work in these areas as it happens in most basic sciences [38]. Hence, by making their work openly accessible, they will enable improvement in all citation-based metrics still narrowly used to evaluate them, freeing time for teaching, sharing of knowledge with the public, writing books, grant proposals, and preparing teaching materials to foster student creativity in the digital age [39].

Inexorably, then, thanks to widespread uptake of OA publishing, research chemists will start to value the benefits of open scholarship including sharing of educational resources [40], thereby dramatically improving outcomes in all three main fields of academic activity: research, education an service to society.

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Notes

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