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Has the time come for preprints in chemistry? A perspective onto a meaningful change

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Abstract
Chemistry is the last natural science discipline to embrace prepublishing, namely the publication of non-peer reviewed scientific articles on the internet. After a brief insight into the origins and the purpose of prepublishing in science, we conduct a concrete analysis of the concrete situation, aiming at providing an answer to several questions. Why the chemistry community has been late in embracing prepublishing? Is this in relation with the slow acceptance of open access publishing by the same community? Will prepublishing become a common habit also for chemistry scholars?

Keywords: prepublishing; preprint; chemistry; open science

Introduction

Communities of computer scientists started to share documents via computer networks in the 1970s.[1] Yet, prepublication of scientific research as we know it today, namely the act to share online a scientific article (a preprint) before the peer review process, debuted in the physics community in 1991 when Ginsparg, a physicist at Los Alamos National Laboratory in the US, released software to share drafts of articles via email transactions referring to a central repository online.[2] Calling them "preprints", Bourne and colleagues recently noted,[3] is an anomaly of language as most of these documents will never have a print version, but only a digital one and most often a DOI (digital object identifier) alphanumeric string.

Pre-publishing their work scholars retain the author rights prior to publication and can subsequently publish their work in any journal accepting prepublished manuscripts. Preprints, in general, are stably archived, dated, and citable, thereby providing evidence for research activity.[4]

With the advent of World Wide Web, the repository for physics articles was first migrated to xxx.lanl.gov and then to arXiv.org, a website managed by the Library of Cornell University. As of June 2017, arXiv hosted more than 1.27 million articles in the fields of physics, mathematics, computer science, quantitative biology, quantitative finance, and statistics, with over 120,000 new submissions expected in 2017.[1]

In late 2013 it was the turn of biologists, who launched bioRxiv.org, a repository for the life sciences research community hosted, again in the US, by Cold Springer Harbor Laboratory. From publishing 824 preprints in the first year,[5] the website has grown to current 1000 monthly submissions,[6] with over 12,000 preprints already archived. In 2016, the engrXiv, SocArxiv and psyArXiv platform were launched to serve, respectively, the engineering, social sciences and psychology communities. So significant has become the impact of preprints, that in 2016 two preprints (the 21st and 28th entries, respectively from bioRxiv and PeerJ Preprints) were in the top 100 list of the most-discussed journal articles of the year produced by Altmetric.[7] More importantly, as emphasized by the founder of arXiv,[2] Perelman's proof of the Poincare conjecture in three dimensions, for which the Russian mathematician was awarded the Fields Medal in 2006, appeared only in three remarkable preprints published in arXiv in 2003. Similarly, Greider regularly publishes her findings in bioRxiv along with other Nobel Prize laureates.

As of July 2017, the Open Science Framework free service had indexed more than 2 million preprints from several disciplines, in fields ranging from architecture to law to education, from such preprint repositories (within brackets the number of preprints) such as AgriXiv (12), arXiv (1,209,405), bioRxiv (12455), BITSS (9), Cogprints (263), engrXiv (115), LawArXiv (194), LIS Scholarship Archive (5), MindRxiv (1), PeerJ (2235), Preprints.org (1765), PsyArXiv (649), RePEc (804,006), SocArXiv (1259).

In chemistry, the reprint server *Nature Precedings* launched in 2007 was closed in 2012 as the website had become "unsustainable as it was originally conceived."[8] A fate shared with the chemistry preprint server launched by Elsevier in year 2000 (along with those in mathematics and computer science) closed in early 2004 as "the Chemistry, Maths and Computer Science research communities did not contribute articles or online comments to the Preprint service in sufficient numbers to justify further development".[9] Twelve years later, in 2016, the American Chemical Society announced the forthcoming launch of ChemRxiv[10] (not yet open for submissions in July 2017),[11] a remarkable change compared to 2000 when, commenting the launch of Elsevier's chemistry preprint server, "nearly all ACS journal editors lined up against it"[12] considering preprints prior publication. Similarly, the Brazilian online publishing platform SciELO announced in early 2017 a forthcoming preprint service.[13]

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Why the chemistry community has been late in embracing prepublishing? Is this in relation with the slow acceptance of open access publishing by the same community? Can we expect widespread acceptance of prepublishing also from chemistry scholars? This study aims to give an answer to these and related questions. After a brief insight into the origins and the purpose of prepublishing in science, we conduct a concrete analysis of the concrete situation, offering an insight into a topic of direct relevance to today's and tomorrow's practitioners of chemical research.

Context, advantages and challenges

A concrete analysis of the concrete situation of prepublishing in chemistry should start from considering the economic relevance of the global scientific publishing industry.[14] This is an industry with total global revenues in 2016 exceeding $24.6 billion, whose profits generally exceed 35% margin.[15] Chemistry is unique among natural sciences because 80% of chemistry papers published in 2006 were published by the five major natural and medical science publishers (American Chemical Society, Reed-Elsevier, Wiley-Blackwell, Springer and Taylor & Francis). The fraction was still above 70% in 2013, whereas it was 40% in 1973 (Figure 1). In physics, for comparison, the proportion of papers published in 2013 by the top five publishers was about 35%.[13]

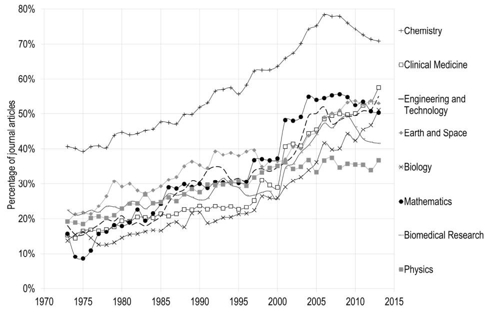

Figure 1. Percentage of papers published by the five major publishers, by discipline in the natural and medical sciences, 1973–2013. [Reproduced from Ref.14, with kind permission].

So far, attempts from public funding agencies to oblige researchers receiving public money to publish only open access articles mostly failed. Only a large private foundation supporting research in life sciences starting in 2017 requires all funded researchers to publish papers uniquely in open access format,[16] thereby excluding journals like *Nature*, *The New England Journal of Medicine*, *Science* and the *Proceedings of the National Academy of Sciences*.

In the early 1990s the advent of the internet first, and of the World Wide Web later, offered an unprecedented opportunity to scholarly communities, namely immediate publication of their findings. Every scholar has gone at least once in her/his career, through the wasteful experience in which the same manuscript was successively rejected and resubmitted until it finds acceptance.[17] Prepublishing has the intrinsic ability to solve the main problem of the peer review process, namely delay in publication.[18] Reducing time to publication can even be of vital importance referring to what happens for instance with research on the Zika virus (a public health emergency) publicly made available in real-time on the Zika Open-Research Portal (https://zika.labkey.com) to help facilitate collaborative research.[9]

Cutting time to publication, prepublication enables researchers to establish priority and, at the same time, share results and data with their colleagues. Scholars immediately start to receive feedback from colleagues who can freely criticize and progress their work. The comments received by other scholars can be used to revise and improve the quality of the original manuscript which often ends published in conventional scientific journals, as it happens to a significant fraction of manuscripts posted on aRxiv, bioRxiv and the other repositories mentioned above. Hence, in principle, the fundamental advantage of prepublishing is the acceleration of scientific and technical progress.

Another key advantage for authors is that they become able to claim priority on new ideas prepublished avoiding plagiarism from unethical referees lamented by several authors: a known misconduct for which the Committee on Publication Ethics (a body established in 1997 by a group of journal editors now having over 10,000 members worldwide from all academic fields) has published guidelines already in 2010.[19] Yet, however untolerable, the latter practice continues to occur even when submitting to high impact factor journals in all sort of disciplines from medicine[20] to chemistry, not only to scientists in their early career, as Noble Prize Lipscomb remarked several years ago:

> «I no longer put my most original ideas in my research proposals, which are read by many referees and officials. I hold back anything that another investigator might hop on and carry out. When I was starting out, people respected each other's research more than they do today, and there was less stealing of ideas».[21]

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Wiersma, a professor of forest resources in the US and the editor of *Environmental Monitoring & Assessment*, argues that the problem with peer review is that it is an “honor system” in which “if people want to break the honor system, there is nothing you can do”.[22]

Today, the problem of plagiarism from unethical referees can be entirely circumvented by prepublishing, especially now that important granting agencies supporting research in life sciences and medicine including the National Institutes of Health in the US,[23] the UK Medical Research Council[24] and Wellcome Trust,[25] almost concomitantly announced in early 2017 new policies for which citation of preprints in grant applications is accepted and even encouraged.

The special case of chemistry

Research chemists have been notoriously reluctant to accept open access (OA) and the number of OA publications in chemistry is still significantly lower than in many other disciplines.[26] Puzzled by such low response of the chemistry community, scientific information scholars have advanced all sort of tentative explanations: from chemistry being a ‘long tail’ science in which small research units would adopt a predominantly non-collaborative mode of research, through the influence of the chemical industry and proprietary information.[27]

In a presentation given at the 2011 Spring meeting of the American Chemical Society, the editors at the first scientific OA publisher in in chemistry (Chemistry Central, founded in 2006, whose parent company BioMed Central was acquired two years later by Springer), noting that acceptance of OA in chemistry was 5 years behind life sciences, suggested one of the main reasons:[28] the influence of chemical Societies, three of which (American Chemical Society, Royal Society of Chemistry, and Germany’s Chemical Society) are among the leading publishers in chemistry, today publishing several OA journals.[29]

In detail, the team showed the outcomes of the EU-funded Study of Open Access Publishing involving 42,000 respondents and 2,300 chemists across the world in which the lowest percentage of researchers who said that OA journals would be beneficial were chemists.[30] In the ranking by country, research chemists based in the United Kingdom (31th out of 33 countries), in the United States (24th) and in Germany (19th) were in the lower part of the ranking.

In brief, interested in their career and in getting funds for their research, the creators of new chemical knowledge had no other option than continuing to publish in journals of renowned reputation so as to increase the impact of their research in terms of citations, and thus their *h*-index and other scientometric indicators to which their promotion and tenure track are closely bound,[31] even though studies showing that OA articles for example in computer science receive significantly more citations than subscription-based articles appeared in prestigious journals as early as of 2001.[32] As the third decade of the 21st century approaches, however, the use of digital prepublishing will become normal also in chemistry, as we critically aim to argument in the following.

A meaningful change

In the last two decades, two significant changes have occurred in communicating chemical research. One is the now complete digitalization of the scientific information flow,[33] with several chemistry journals no longer printing journal issues but producing only articles in digital format (normally in both portable document format, PDF, and HTML). Another is the now predominant use of the World Wide Web to search for scientific information,[34] especially through free search services such as those offered by Google Scholar. The latter search engine, furthermore, effectively tracks citation of researchers who use it also for getting updated scientometric information of relevance to their own curriculum.[35]

From *Chemical Communications* to *Organic Letters*, numerous prestigious journals are available to chemists to quickly publish findings of high relevance, and even in OA format when paying the article processing charge. However, the same is true for biology and physics where numerous journals, including new “express” “protocols” and “letters” versions of prestigious titles, offer a fast track to peer reviewed publication, but this has not slowed down acceptance of prepublishing in those communities. Chemical researchers too will shortly start to use prepublishing to claim priority for their findings, share them and get feedback in matter of days or weeks, rather than in months or years as it used to be with conventional publishing. For those who will stick to the old model, the risk is to see colleagues prepublishing their work in the same sub-field of contemporary chemical research to rapidly progress the field while they are still waiting months for the reviewers’ reports.

This is also what happened in the biology community, which came to prepublishing about two decades after physics. The information specialist arguing in early 2016 to be curious “to see if bioRxiv continues to see its submissions grow”,[9] one year later saw the number of prepublished articles in bioRxiv surpassing the 12,000 threshold (from less 900 in the first year). This may explain why large publishers have recently started new preprint repository services, such as for example Preprints owned by MDPI; and it may also explain why arXiv[36] and bioRxiv[37] are frequently used also by chemists, often for papers jointly authored with physicists or life scientists. Gone are the days when chemistry preprint servers were closed due to insufficient submissions.

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Joining the open science practice, chemists and especially young chemical research practitioners, will discover or re-discover that, as put it by Nosek, a social psychologist and open science advocate, "sharing is good", *i.e.* sharing research with peers is good for discovery;[38] restoring the original meaning of scientific publication vividly illustrated by Evariste Galois, the eminent mathematician creator of the Group theory, in 1831:

> «*Je rêve d'un temps où l'égoïsme ne régnera plus dans les sciences, où on s'associera pour étudier, au lieu d'envoyer aux académies des plis cachetés, on s'empressera de publier ses moindres observations pour peu qu'elles soient nouvelles, et on ajoutera: 'Je ne sais pas le reste'*».[39]

Whether or not prepublishing and open access will enable to get rid of egoism in science, as auspicated by Galois, interest for promotion and research funds perhaps will. Following the recent decision of the world's largest science funding agency (NIH, funding research with >$26 billion in 2013),[40] other scientific funding agencies worldwide will approve citation of preprints in the grant applications, including those supporting research in chemistry.

By then, promotion, search and tenure committees will do the same, accepting citation of preprints in the curriculum of applicants, after having adopted clear policies on how preprints should be evaluated. "Non-refereed publications, for example on pre-print servers, should be clearly classified as such", lately wrote the director of Germany's Chemical Society.[41] Since the early days of prepublishing, however, preprints were, and still are, explicitly identified as such.

Outlook and Perspectives

Echoing the title the work of geneticist Bhalla for biology,[42] this work aims to answer the question whether the time has come for prepublishing in chemistry. Though being the last discipline among natural sciences to embrace prepublishing, chemistry nonetheless in the last two decades has undergone through a first significant change in the communication process which has dominated the central science for more than a century, with the now complete digitalization of the scientific information flow.

Interested in their career and in getting research funds, chemistry researchers cannot ignore any longer prepublishing as the vast majority of them did with open access journals. Preprints are cited, and their citation counted by academic and scholar search engines *and* accepted and even encouraged by public funding agencies, starting from the world's largest (the NIH) and soon by many others across the world. Fully indexed, preprints provide researchers with visibility in the research community enabling them, for instance, to easily access online the article metrics and see all referrers.[43]

From the fundamental viewpoint of research practice, the benefits of immediate feedback on the published research from a much wider audience (online preprints can be freely accessed and downloaded) are so significant that research chemists competing for priority in discovery and innovation will increasingly prepublish their findings as a normal part of the research communication process. Prepublishing, indeed, has the intrinsic ability to address the major problem of the peer review process, *i.e.* the exceedingly long time between submission and publication.

Also in chemistry, the relationship between journals and preprint servers will likely be of symbiotic nature, with editors browsing preprint servers looking for suitable articles likewise to what the editors of *PLOS Genetics*[44] and *Genome Biology*[45] currently do, soliciting authors to submit their preprints for peer review and, increasingly, for open peer review.[18] To compete with numerous prestigious journals such as *PLoS One* accepting prepublished manuscripts for peer-review, chemistry journals which currently do not accept prepublished manuscripts will shortly change their policies towards prepublication, as it already happened at several ACS journals where the decision is left to the journal editors.

At the 2017 Lindau Meeting of Nobel Laureates, Chalfie lately informed the audience that periodically a member of his research group is required to select a preprint on a topic related to her/his research.[46] The study is discussed in a subsequent group meeting, and comments are eventually sent to the preprint corresponding author in order to raise new ideas both in Chalfie's group as well as in that of the author.

Why research groups in chemistry should not adopt similar practices? Is there anyone in the chemistry community who really agrees with the viewpoint that chemists would adopt a "predominantly noncollaborative mode of research" which "reduces the incentive to make use of new technologies to facilitate data sharing and research collaboration"?[27]

In China, where chemistry in 2014 accounted for 61% of the country's total weighted fractional count,[47] collaborations in the field of chemistry soared to unprecedented levels, with major collaborations in 2015 with groups based in the US, Germany, Japan, Singapore, UK, Australia, Canada and France.[48]

To survive, preprint servers will need financial revenues. Hence, they will be owned from existing publishers (like Preprints), from public research bodies (like arXiv or bioRxiv), from private foundations (as it happens with the *Beilstein Journal of Organic Chemistry* journal) or even by public or private funders of research. Whatever their ownership, however, preprint servers will continue to thrive and improve becoming of central relevance in the new way to communicate innovation in science, and also in

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chemistry. The process is underway, and this study will hopefully assist research chemists in the transition to open science for the benefit of the main users of chemical innovation: mankind.

Author contribution

M.P. co-conceived the manuscript, analysed the data, interpreted the results and wrote the manuscript. R.C. and P.D.C. co-conceived the manuscript, collected the data, interpreted the results and revised the manuscript. All authors gave final approval for publication.

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