

# Writing Journal Articles

C. David Sherrill

School of Chemistry and Biochemistry

Georgia Institute of Technology

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## 1 Introduction

These notes include some advice on how to write a paper for publication in a peer-reviewed journal. Considerably more extensive advice on this subject is available in other sources such as the *ACS Style Guide*.

## 2 Goals for a Paper

As Fritz Schaefer used to say, “if it isn’t published, it doesn’t exist.” Although you might present unpublished work as a poster or a talk, only a publication will elevate it to the status of a legitimate, completed project worthy of discussion. Your publication list is one of the most important items on your curriculum vitae. The first goal for a paper, then, is to conclude a project and earn credit for the work.

To achieve the first goal, it is necessary to write a paper that will pass peer review. A paper that is clear and well-organized is more likely to be accepted for publication. Journals also only want to publish original research that will have a significant impact. Therefore it is necessary to explain how your paper differs from previous work, why your paper is important, and what new insights it presents.

The second goal for a paper is to inform the community about what you have done and why it is important. The most successful publications are those that teach others about a new discovery or a new way of looking at things. This enhances the ability of other researchers to make progress in their own projects. In more applied areas of research, published research may ultimately result in new products, devices, diagnostic procedures, etc., that can benefit society.

To achieve the second goal, you need to decide what audience you wish to reach, and write the paper appropriately. This also affects the choice of the journal to which the paper should be submitted.

Finally, a paper should have one major point, or one main thing that it is about. Trying to accomplish too much in one paper can dilute your message and make it harder for readers to understand what the paper was about.

## **3 Parts of the Paper**

### **3.1 Abstract**

This should be an extremely concise summary of the major findings of the article. It should not be more than 150 words, and some journals have hard limits on the number of words allowed. The abstract is not merely an advertisement for the article — the main results should be presented directly in the abstract to the extent possible within the space allowed.

### **3.2 Introduction**

This is the part where you explain why your paper is interesting. It should set up the problem, including a thorough discussion of the literature. The last part of the introduction should give a *very* brief idea (no more than a paragraph) about what is discovered in the paper. During peer review, the referees (and often the editor) will focus on the introduction and conclusions when they are trying to figure out what the paper is about, and if its findings are important.

### **3.3 Methods**

For theorists, this section may also be called “Theoretical Methods.” In this section, explain *how* you did what you did. You should give sufficient detail that anyone else who is properly trained in your subfield should be able to reproduce your results. For routine applications of standard methods, this part should be as clear and concise as possible, usually 2-4 paragraphs. For papers describing the development of new theoretical approaches, this is usually the bulk of the paper, and typically there are multiple sections describing each part of the theory, with no section called “Methods.”

### **3.4 Results and Discussion**

It is possible to split this into two sections, but more frequently they are combined. This section should introduce the results and then discuss what they mean, why they are what they are, and what consequences they have. This section contains the meat of the paper and should cover any details not already explained in the methods section.

### **3.5 Conclusions**

This section, of perhaps 1-3 paragraphs, should briefly summarize what the paper has discovered and go on to state the broader significance of these findings. The main point of the paper should be stated or re-stated here.

## 4 Figures

For simpler figures consisting of lines, circles, etc., it is optimal to use “vector graphics,” which consist of a set of instructions for drawing the figure (e.g., draw a line from here to here). This allows the figure to scale well to any size. Adobe Illustrator is an example of a program that can create vector graphics, and they are often written out in Postscript or PDF format. Text always looks much better in a vector graphics format, because it often doesn’t scale well to other sizes.

For all other figures, a “bit-mapped” format (storing individual pixels) is ok if a high resolution is used (typically 300 dpi is desirable; do not go to super high resolutions like 1200 dpi, it will make the file too large to deal with easily). Examples of bit-mapped file formats are PNG, JPEG, etc.

When you are creating figures, try to initially create them in the size they will have in the final published article. For example, if you want a small single-column figure, do not initially create it as a full-page figure and then try to scale it down later. Sometimes the scaling process yields undesirable bad results (especially for bit-mapped figures).

Avoid very tiny symbols or fonts, or tiny dashes in lines. These are hard to read for a reader. *A figure must be easy on the reader, not hard to see or read or understand.*

Please refer to <http://vergil.chemistry.gatech.edu/resources/figures.html> for more information.

## 5 General Suggestions

Throughout the paper, the following general rules should be helpful:

1. Be concise. Don’t say more than you need, except as required by the other rules.
2. Be correct. If you say your data agree with experiment within 10%, but one of the data points has an error of 11%, then the statement is not actually correct. Try to avoid making statements that are generally but not always true.
3. Be clear. Don’t write something that the average reader won’t understand.
4. Be relevant. Try to avoid discussions about issues that aren’t related to the point of the paper.

## 6 Tips for General Scientific Papers

1. *Important!* For journals that use citation numbers as superscripts, the superscript comes *after* the punctuation. For example: We follow the notation of Handy *et al.*<sup>4</sup>
2. Avoid superscripts on numbers, because they’ll look like exponents. For example, “the mean absolute error for this method is 0.28<sup>13</sup> kcal mol<sup>-1</sup>.”

3. *Introduce all acronyms the first time they are used. Copy editors will insist on this very strictly, so this is something you will not be able to avoid — just go ahead and get it right in the draft before sending the draft to your advisor.*
4. Avoid use of acronyms in titles. Possible rare exceptions might include the introduction of a new method/acronym, or cases where the acronym is much more recognizable than the full name. Any acronyms used in titles should be spelled out.
5. The Latin phrase “*et al.*” is short for “*et alia*,” which means “and the others.” The *et* does not have a period because it is not abbreviated.
6. If you wish to refer to a paper with only two authors, do not use *et al.* Instead, list both authors (e.g., “Sinnokrot and Sherrill”).
7. For papers with more than two authors, you may refer to the paper using the last name of the first author plus “*et al.*” (for example, “Sinnokrot *et al.*”), OR using the last name of the corresponding author plus “and co-workers” (for example, “Head-Gordon and co-workers”).
8. Try to avoid repeating a word or phrase within a sentence or pair of sentences.
9. Don’t use the same sentence more than once in your paper.
10. Don’t have a sentence that says basically the same thing as the previous sentence (unless you are explaining something tricky and technical by saying it in other words).
11. Don’t use the word “numbers” in a context where you mean “values,” e.g., don’t say “Our results are more reliable than the previously reported numbers.”
12. Avoid the phrase “we looked at.” Try “we considered.”
13. Try to give an appropriate number of digits in tables, etc. Don’t give more digits than are significant.
14. *Which vs. That:* Use “that” to define a subset, and “which” to clarify all items of a set. For example, “We toured castles that had moats,” uses *that* because not all castles have moats. On the other hand, “We used NMR, which is a spectroscopic technique.”
15. *Punctuation:* Use commas when a pause in the sentence is called for. Use a semicolon (;) before introducing a new independent clause in a sentence. Use a colon (:) before introducing a clarifying comment or a list (e.g., “there are three main approaches: x, y, and z.”) A semicolon can be used to separate items in a list if the items themselves contain commas (e.g., “three approaches: density functional theory, with whatever functionals are deemed sufficiently accurate; second-order perturbation theory; and coupled-cluster theory.”)

16. Use square brackets instead of parentheses if you would otherwise have parentheses within parentheses: e.g., “coupled-cluster theory with perturbative triple substitutions [CCSD(T)].” (This comment pertains primarily to main text, not always to equations).
17. Chemical formulas are written in Roman type, not italics: CH<sub>4</sub>, not *CH*<sub>4</sub>.
18. Equations are punctuated like sentences. Equations in the middle of a sentence get a comma after them, and equations that end sentences end with a period.
19. Use abbreviated forms of units of measurement (mL not milliliter), use a space between quantity and unit (5 mL not 5mL). Do not pluralize units unless they are spelled out. I prefer kcal mol<sup>-1</sup> to kcal/mol, and to spell out Hartrees.
20. Variables should be in italics or math type, and labels should be in Roman type. For example, a dissociation energy is  $D_0$ , but an electrostatic energy might be denoted  $E_{\text{elst}}$  (with the extended “label” elst in Roman type).
21. Define all symbols used in all equations, unless they are widely recognized. The symbols should be defined immediately after they are used in the equation (if they haven’t already been defined).

## 7 Tips for Theoretical Chemistry Papers

1. Try to use “computations,” instead of “calculations.” Especially avoid the phrase “ran calculations.”
2. A “level of theory” refers to a combination of a basis set and a correlation method. You might say “computed at the MP2/6-31G\* level of theory,” but avoid saying “computed at the MP2 level of theory.”
3. If you say you “used the 6-31G\*\* method,” this signals a lack of familiarity with computational chemistry. 6-31G\*\* is a basis set, not a method.
4. For relative energies in kcal mol<sup>-1</sup>, often 1-3 digits after the decimal is appropriate. If the theoretical methods used are not particularly accurate for the quantity being computed (e.g., DFT barrier heights), then you might want to report relative energies only to 0.1 kcal mol<sup>-1</sup>.
5. Six digits is usually a good number for total electronic energies, even if there are more significant digits than this. However, total energies are boring, and you probably don’t want to report them in a normal paper, except perhaps in the SI. If they are in a table inside the SI, then go ahead and format to 6 digits. If they are in some data file, then there’s no good reason to truncate them at 6 digits and you can go ahead and use however many digits you have.

6. When you compare X to Y, make the Y the more accurate value; we compare DFT to experiment, we don't compare experiment to DFT
7. Avoid using program-specific keywords in the Methods section, when possible; instead, provide the values of the relevant cutoffs in a way that could be used for other programs also

## 8 Special Considerations for L<sup>A</sup>T<sub>E</sub>X

1. Avoid defining new commands for convenience (e.g., with `newcommand`). This causes problems with the type conversion software used by the Journals.
2. Quotation marks are handled in a funny way in L<sup>A</sup>T<sub>E</sub>X. Depending on the version of L<sup>A</sup>T<sub>E</sub>X, the double-quotes keyboard character will not necessarily render correctly into a good-looking open-double-quotes or end-double-quotes. Create an opening double-quotes mark by two single open-quote marks (using the keyboard key that also has a tilde on it): ‘‘. This should render as “. Create a closing double-quotes mark by two single end-quote marks (using the keyboard key next to Enter that also has a double-quotes mark on it): ’’. This should render as ”.
3. Some versions of L<sup>A</sup>T<sub>E</sub>X need to be told if a period is ending a sentence or not. Otherwise, they will assume all periods end a sentence, and it will put extra space after it, which is not always appropriate. For example, the following sentence looks funny because there is too much space after the period in “et al.”:

Schaefer et al. showed that

We can fix this by adding a slash or tilde character after the period (`.\` or `.~`):

Schaefer et al. showed that