

Template for preparing your Brief Report submission to PNAS using Overleaf

Author One^{a,c,1}, Author Two^{b,1,2}, and Author Three^a

^aAffiliation One; ^bAffiliation Two; ^cAffiliation Three

This manuscript was compiled on July 8, 2019

1 Please provide an abstract of no more than 250 words in a single
2 paragraph. Abstracts should explain to the general reader the major
3 contributions of the article. References in the abstract must be cited
4 in full within the abstract itself and cited in the text.

Keyword 1 | Keyword 2 | Keyword 3 | ...

1 This PNAS journal template is provided to help you write
2 your work in the correct journal format. Instructions for
3 use are provided below.

4 Note: please start your introduction without including the
5 word “Introduction” as a section heading (except for math arti-
6 cles in the Physical Sciences section); this heading is implied
7 in the first paragraphs.

8 Guide to using this template on Overleaf

9 Please note that whilst this template provides a preview of the
10 typeset manuscript for submission, to help in this preparation,
11 it will not necessarily be the final publication layout. For
12 more detailed information please see the [PNAS Information
13 for Authors](#).

14 If you have a question while using this template on Overleaf,
15 please use the help menu (“?”) on the top bar to search for [help
16 and tutorials](#). You can also [contact the Overleaf support team](#)
17 at any time with specific questions about your manuscript or
18 feedback on the template.

19 **Author Affiliations.** Include department, institution, and com-
20 plete address, with the ZIP/postal code, for each author. Use
21 lower case letters to match authors with institutions, as shown
22 in the example. Authors with an ORCID ID may supply this
23 information at submission.

24 **Submitting Manuscripts.** All authors must submit their arti-
25 cles at [PNAScentral](#). If you are using Overleaf to write your
26 article, you can use the “Submit to PNAS” option in the top
27 bar of the editor window.

28 **Format.** Many authors find it useful to organize their
29 manuscripts with the following order of sections; Title, Au-
30 thor Affiliation, Keywords, Abstract, Introduction, Results,
31 Discussion, Materials and methods, Acknowledgments, and
32 References. Other orders and headings are permitted.

33 **Manuscript Length.** PNAS generally uses a two-column for-
34 mat averaging 67 characters, including spaces, per line. The
35 maximum length of a Brief Report article is 18,000-20,000
36 characters, including all text, spaces, and the number of char-
37 acters displaced by equations and graphical elements. Brief
38 Reports should be no longer than 2,000 words.

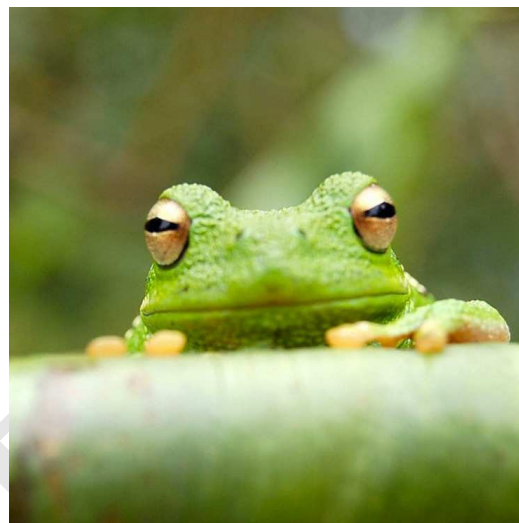


Fig. 1. Placeholder image of a frog with a long example caption to show justification setting.

References. References should be cited in numerical order as they appear in text; this will be done automatically via bibtex, e.g. (1) and (2, 3). All references cited in the main text should be included in the main manuscript file.

Data Archival. PNAS must be able to archive the data essential to a published article. Where such archiving is not possible, deposition of data in public databases, such as GenBank, ArrayExpress, Protein Data Bank, Unidata, and others outlined in the Information for Authors, is acceptable.

Language-Editing Services. Prior to submission, authors who believe their manuscripts would benefit from professional editing are encouraged to use a language-editing service (see list at www.pnas.org/site/authors/language-editing.xhtml). PNAS does not take responsibility for or endorse these services, and their use has no bearing on acceptance of a manuscript for publication.

Digital Figures. Only TIFF, EPS, and high-resolution PDF for Mac or PC are allowed for figures that will appear in the main text, and images must be final size. Authors may submit U3D or PRC files for 3D images; these must be accompanied by 2D representations in TIFF, EPS, or high-resolution PDF

Please provide details of author contributions here.

Please declare any conflict of interest here.

¹A.O.(Author One) and A.T. (Author Two) contributed equally to this work (remove if not applicable).

²To whom correspondence should be addressed. E-mail: author.twoemail.com

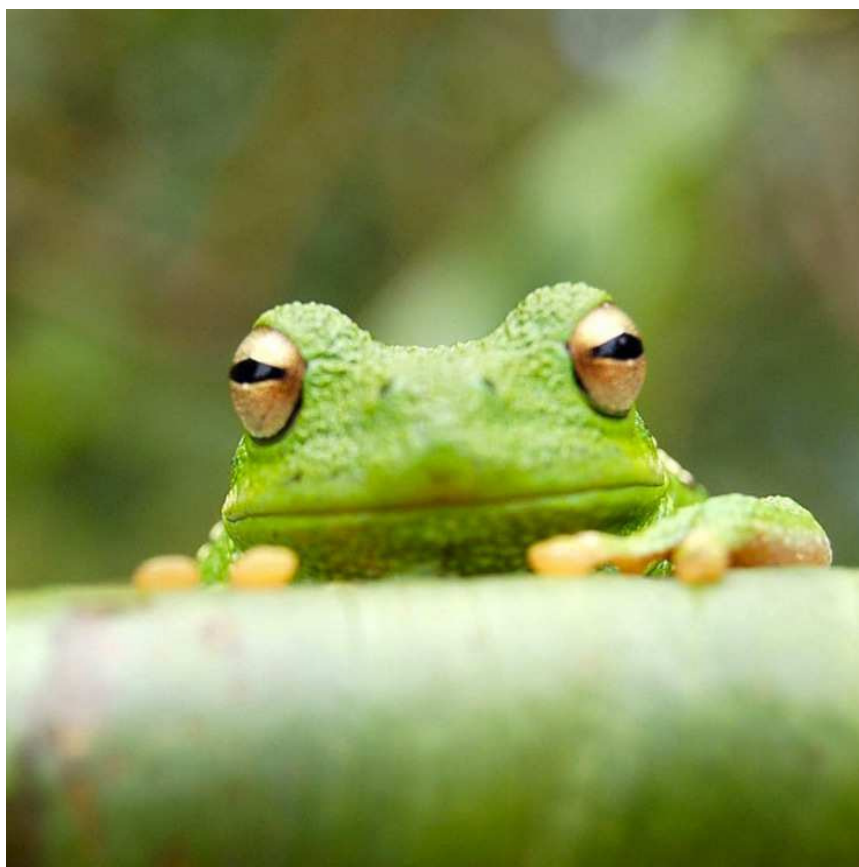


Fig. 2. This caption would be placed at the side of the figure, rather than below it.

$$\begin{aligned}
 (x + y)^3 &= (x + y)(x + y)^2 \\
 &= (x + y)(x^2 + 2xy + y^2) \\
 &= x^3 + 3x^2y + 3xy^2 + y^3.
 \end{aligned}
 \tag{1}$$

60 format. Color images must be in RGB (red, green, blue) mode.
 61 Include the font files for any text.

62 Figures and Tables should be labelled and referenced in the
 63 standard way using the `\label{}` and `\ref{}` commands.

64 Figure 1 shows an example of how to insert a column-wide
 65 figure. To insert a figure wider than one column, please use
 66 the `\begin{figure*}... \end{figure*}` environment. Fig-
 67 ures wider than one column should be sized to 11.4 cm or 17.8
 68 cm wide. Use `\begin{SCfigure*}... \end{SCfigure*}` for a
 69 wide figure with side captions.

70 **Tables.** Tables should be included in the main manuscript file
 71 and should not be uploaded separately.

72 **Single column equations.** Authors may use 1- or 2-column
 73 equations in their article, according to their preference.

74 To allow an equation to span both columns, use the
 75 `\begin{figure*}... \end{figure*}` environment mentioned
 76 above for figures.

77 Note that the use of the `widetext` environment for equa-
 78 tions is not recommended, and should not be used.

79 **Supporting Information (SI).** Authors are limited to the follow-
 80 ing types of SI: datasets, videos, and 3D figures. Extended

Table 1. Comparison of the fitted potential energy surfaces and ab initio benchmark electronic energy calculations

Species	CBS	CV	G3
1. Acetaldehyde	0.0	0.0	0.0
2. Vinyl alcohol	9.1	9.6	13.5
3. Hydroxyethylidene	50.8	51.2	54.0

nomenclature for the TSs refers to the numbered species in the table.

methods or discussion are not permitted.

SI Datasets. Supply .xlsx, .csv, .txt, .rtf, or .pdf files. This file
 type will be published in raw format and will not be edited or
 composed.

SI Movies. Supply Audio Video Interleave (avi), Quicktime
 (mov), Windows Media (wmv), animated GIF (gif), or MPEG
 files and include a brief legend for each movie in the main
 manuscript file. All movies should be submitted at the desired
 reproduction size and length. Movies should be no more than
 10 MB in size.

3D Figures. Supply a composable U3D or PRC file so that it
 may be edited and composed. Authors may submit a PDF file

93 but please note it will be published in raw format and will not
94 be edited or composed.

95 **Materials and Methods**

96 Please describe your materials and methods here. This can be more
97 than one paragraph, and may contain subsections and equations
98 as required. Authors should include a statement in the methods
99 section describing how readers will be able to access the data in the
100 paper.

101 **Subsection for Method.** Example text for subsection.

102 **ACKNOWLEDGMENTS.** Please include your acknowledgments
103 here, set in a single paragraph. Please do not include any acknowl-
104 edgments in the Supporting Information, or anywhere else in the
105 manuscript.

- 106 1. M Belkin, P Niyogi, Using manifold structure for partially labeled classification in *Advances in*
107 *neural information processing systems*. pp. 929–936 (2002).
- 108 2. P Bérard, G Besson, S Gallot, Embedding riemannian manifolds by their heat kernel. *Geom.*
109 *& Funct. Analysis GAFA* **4**, 373–398 (1994).
- 110 3. RR Coifman, et al., Geometric diffusions as a tool for harmonic analysis and structure definition
111 of data: Diffusion maps. *Proc. Natl. Acad. Sci. United States Am.* **102**, 7426–7431 (2005).

DRAFT