

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 May 14, 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 **T**his 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 format
 34 averaging characters, including spaces, per line. The maxi-
 35 mum length of a Brief Report article is 3 pages including all
 36 text, spaces, and the number of characters displaced by fig-
 37 ures, tables, and equations. When submitting tables, figures,
 38 and/or equations in addition to text, keep the total number of
 39 characters (including spaces) to under 15,000. Brief Reports
 40 should be no longer than 2,000 words.

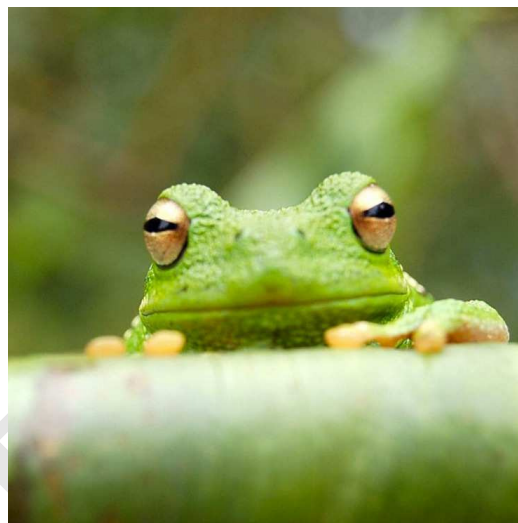


Fig. 1. Placeholder image of a frog with a long example caption to show justification setting.

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, Ar-
 rayExpress, 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 edit-
 ing 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
 format. Color images must be in RGB (red, green, blue) mode.
 Include the font files for any text.

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

Figure 1 shows an example of how to insert a column-wide
 figure. To insert a figure wider than one column, please use

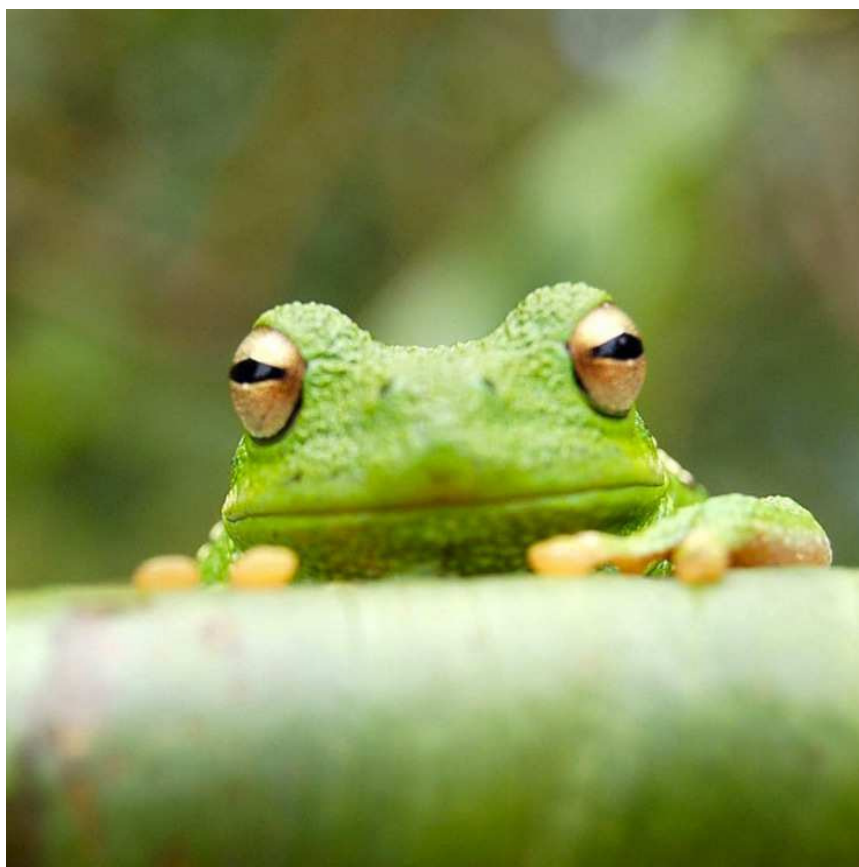


Fig. 2. This caption would be placed at the side of the figure, rather than below it.

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

the `\begin{figure*}... \end{figure*}` environment. Figures wider than one column should be sized to 11.4 cm or 17.8 cm wide. Use `\begin{SCfigure*}... \end{SCfigure*}` for a wide figure with side captions.

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

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

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

Note that the use of the `widetext` environment for equations is not recommended, and should not be used.

Supporting Information (SI). Authors are limited to the following types of SI: datasets, videos, and 3D figures. Extended 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.

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.

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

97 **Materials and Methods**

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

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

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

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

DRAFT