

Template for preparing your research 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 September 29, 2020

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. PNAS strongly encourages authors to sup-
23 ply an [ORCID identifier](#) for each author. Individual authors
24 must link their ORCID account to their PNAS account at
25 [www.pnascentral.org](#). For proper authentication, authors must
26 provide their ORCID at submission and are not permitted to
27 add ORCIDs on proofs.

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

32 **Format.** Many authors find it useful to organize their
33 manuscripts with the following order of sections; title, author
34 line and affiliations, keywords, abstract, significance statement,
35 introduction, results, discussion, materials and methods, ac-
36 knowledgments, and references. Other orders and headings
37 are permitted.

38 **Manuscript Length.** A standard 6-page article is approximately
39 4,000 words, 50 references, and 4 medium-size graphical el-
40 ements (i.e., figures and tables). The preferred length of

articles remains at 6 pages, but PNAS will allow articles up
to a maximum of 12 pages.

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/page/authors/language-editing](#)). PNAS does
not take responsibility for or endorse these services, and their
use has no bearing on acceptance of a manuscript for publica-
tion.

Digital Figures. EPS, high-resolution PDF, and PowerPoint
are preferred formats for figures that will be used in the main
manuscript. Authors may submit PRC or U3D 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.

Images must be provided at final size, preferably 1 column
width (8.7cm). Figures wider than 1 column should be sized
to 11.4cm or 17.8cm wide. Numbers, letters, and symbols
should be no smaller than 6 points (2mm) and no larger than
12 points (6mm) after reduction and must be consistent.

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

Significance Statement

Authors must submit a 120-word maximum statement about the significance of their research paper written at a level understandable to an undergraduate educated scientist outside their field of speciality. The primary goal of the significance statement is to explain the relevance of the work in broad context to a broad readership. The significance statement appears in the paper itself and is required for all research papers.

Please provide details of author contributions here.

Please declare any competing interests here.

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

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

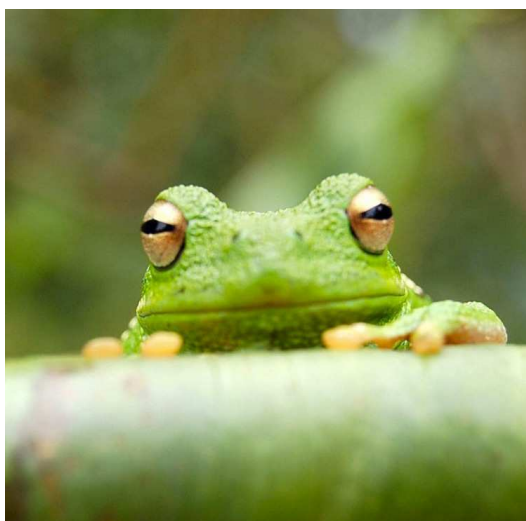


Fig. 1. Placeholder image of a frog with a long example legend to show justification setting.

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.

73 Figure 1 shows an example of how to insert a column-wide
 74 figure. To insert a figure wider than one column, please use
 75 the `\begin{figure*}... \end{figure*}` environment. Fig-
 76 ures wider than one column should be sized to 11.4 cm or 17.8
 77 cm wide. Use `\begin{SCfigure*}... \end{SCfigure*}` for a
 78 wide figure with side legends.

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

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

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

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

88 **Supporting Information Appendix (SI).** Authors should submit
 89 SI as a single separate SI Appendix PDF file, combining all
 90 text, figures, tables, movie legends, and SI references. SI
 91 will be published as provided by the authors; it will not be
 92 edited or composed. Additional details can be found in the
 93 [PNAS Author Center](#). The PNAS Overleaf SI template can
 94 be found [here](#). Refer to the SI Appendix in the manuscript at
 95 an appropriate point in the text. Number supporting figures
 96 and tables starting with S1, S2, etc.

97 Authors who place detailed materials and methods in an
 98 SI Appendix must provide sufficient detail in the main text
 99 methods to enable a reader to follow the logic of the procedures
 100 and results and also must reference the SI methods. If a paper

is fundamentally a study of a new method or technique, then
 the methods must be described completely in the main text.

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. Movie legends should be included in the SI Appendix file.
 All movies should be submitted at the desired reproduction
 size and length. Movies should be no more than 10MB 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.

Materials and Methods

Please describe your materials and methods here. This can be more
 than one paragraph, and may contain subsections and equations as
 required.

Subsection for Method. Example text for subsection.

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

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

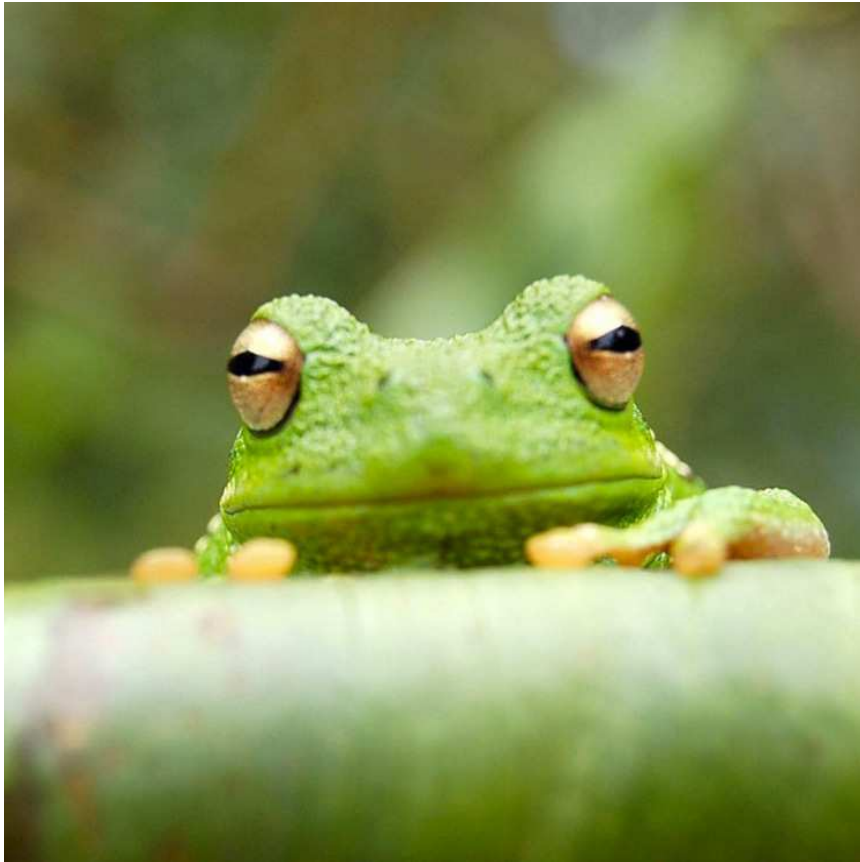


Fig. 2. This legend would be placed at the side of the figure, rather than below it.

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