42

43

45

46

47

50

51

53

54

55

58

59

60

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

^a Affiliation One; ^b Affiliation Two; ^c Affiliation Three

This manuscript was compiled on October 28, 2019

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

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

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

Note: please start your introduction without including the word "Introduction" as a section heading (except for math articles in the Physical Sciences section); this heading is implied in the first paragraphs.

Guide to using this template on Overleaf

13

21

22

33

Please note that whilst this template provides a preview of the typeset manuscript for submission, to help in this preparation, it will not necessarily be the final publication layout. For more detailed information please see the PNAS Information for Authors.

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

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

Submitting Manuscripts. All authors must submit their articles at PNAScentral. If you are using Overleaf to write your article, you can use the "Submit to PNAS" option in the top bar of the editor window.

Format. Many authors find it useful to organize their manuscripts with the following order of sections; title, author line and affiliations, keywords, abstract, introduction, results, discussion, materials and methods, acknowledgments, and references. Other orders and headings are permitted.

Manuscript Length. The maximum length of a Brief Report article is 20,000 characters, including all text, spaces, and the number of characters displaced by equations and graphical elements. Brief Reports typically include no more than 2 graphical elements (e.g., figures and tables) and Supporting Information is limited to essential supporting datasets and videos; additional methods, tables, or figures are not permit-



Fig. 1. Placeholder image of a frog with a long example legend 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/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 publication.

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

Please provide details of author contributions here.

Please declare any competing interests here.

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

 $^{^2\}mathrm{To}$ whom correspondence should be addressed. E-mail: author.twoemail.com



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

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.

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

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.

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

Species	CBS	CV	G3
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 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 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.

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. Authors should include a statement in the methods 98

99

100

101

102

103

63

64

65

66

67

68

71

72

73

74

75

78

81

82

83

$$(x+y)^3 = (x+y)(x+y)^2$$

= $(x+y)(x^2 + 2xy + y^2)$
= $x^3 + 3x^2y + 3xy^3 + x^3$. [1]

- $_{\rm 106}$ $\,$ section describing how readers will be able to access the data in the $_{\rm 107}$ $\,$ paper.
- 108 Subsection for Method. Example text for subsection.
- ACKNOWLEDGMENTS. Please include your acknowledgments here, set in a single paragraph. Please do not include any acknowledgments in the Supporting Information, or anywhere else in the manuscript.
- M Belkin, P Niyogi, Using manifold stucture for partially labeled classification in Advances in neural information processing systems. pp. 929–936 (2002).
- P Bérard, G Besson, S Gallot, Embedding riemannian manifolds by their heat kernel. *Geom.* & Funct. Analysis GAFA 4, 373–398 (1994).
- 117 3. RR Coifman, et al., Geometric diffusions as a tool for harmonic analysis and structure definition
 118 of data: Diffusion maps. Proc. Natl. Acad. Sci. United States Am. 102, 7426–7431 (2005).