## Template for preparing your research report submission to PNAS

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

<sup>a</sup> Affiliation One; <sup>b</sup> Affiliation Two; <sup>c</sup> Affiliation Three

This manuscript was compiled on January 6, 2023

- Please provide an abstract of no more than 250 words in a single paragraph. Abstracts should explain to the general reader the major
- 3 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 | ...

his 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

11

12

20

21

22

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 Affiliation, Keywords, Abstract, Significance Statement, Results, Discussion, Materials and methods, Acknowledgments, and References. Other orders and headings are permitted.

Manuscript Length. PNAS generally uses a two-column format averaging 67 characters, including spaces, per line. The maximum length of a Direct Submission research article is six pages and a Direct Submission Plus research article is ten pages including all text, spaces, and the number of characters displaced by figures, tables, and equations. When submitting tables, figures, and/or equations in addition to text, keep the text for your manuscript under 39,000 characters (including spaces) for

Direct Submissions and 72,000 characters (including spaces) for Direct Submission Plus.

41

42

44

45

46

47

49

50

51

52

53

55

56

57

58

60

61

62

63

64

65

68

70

71

72

73

**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 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 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 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.

## **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 conflict of interest here.

<sup>&</sup>lt;sup>1</sup>A.O.(Author One) and A.T. (Author Two) contributed equally to this work (remove if not applicable).

<sup>&</sup>lt;sup>2</sup>To whom correspondence should be addressed. E-mail: author.twoemail.com



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

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  |
| <ol><li>Vinyl alcohol</li></ol> | 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.

**Tables.** In addition to including your tables within this manuscript file, PNAS requires that each table be uploaded to the submission separately as a "Table" file. Please ensure that each table .tex file contains a preamble, the \begin{document} command, and the \end{document} command. This is necessary so that the submission system can convert each file to PDF.

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 should submit SI as a single separate PDF file, combining all text, figures, tables, movie legends, and SI references. PNAS will publish SI uncomposed, as the authors have provided it. Additional details can be found here: policy on SI. For SI formatting instructions click here. The PNAS Overleaf SI template can be found here. Refer to the SI Appendix in the manuscript at an appropriate point in the text. Number supporting figures and tables starting with S1, S2, etc.

Authors who place detailed materials and methods in an SI Appendix must provide sufficient detail in the main text methods to enable a reader to follow the logic of the procedures 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 Excel (.xls), RTF, or PDF files. This file type will be published in raw format and will not be edited or composed.

103

104

105

106

108

109

110

111

112

113

114

115

116

117

118

119

120 121

122

123

124

125

126

127

128

129

130

131

132

133

SI Movies. Supply Audio Video Interleave (avi), Quicktime (mov), Windows Media (wmv), animated GIF (gif), or MPEG files and submit a brief legend for each movie in a Word or RTF 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 section describing how readers will be able to access the data in the

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.

- 1. Belkin M, Niyogi P (2002) Using manifold stucture for partially labeled classification in Advances in neural information processing systems. pp. 929-936.
- Bérard P, Besson G, Gallot S (1994) Embedding riemannian manifolds by their heat kernel. Geometric & Functional Analysis GAFA 4(4):373-398.
- Coifman RR, et al. (2005) Geometric diffusions as a tool for harmonic analysis and structure definition of data: Diffusion maps. Proceedings of the National Academy of Sciences of the United States of America 102(21):7426-7431.

2 | www.pnas.org/cgi/doi/10.1073/pnas.XXXXXXXXXX

75

79

80

82

83

84

85

86

87

88

89

90

91

92

95

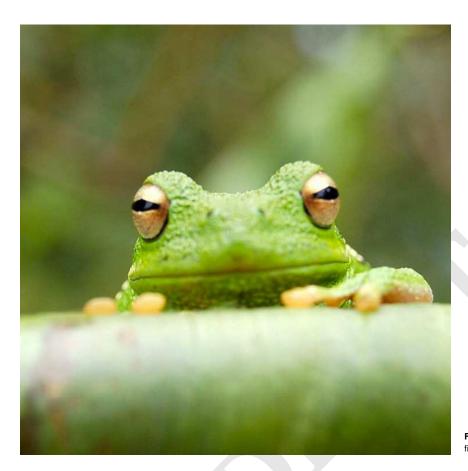
96

97

98

99

100



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

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

$$= (x+y)(x^{2} + 2xy + y^{2})$$

$$= x^{3} + 3x^{2}y + 3xy^{3} + x^{3}.$$
[1]

Lead author last name et al. PNAS | January 6, 2023 | vol. XXX | no. XX | 3