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Author One a,c,1, Author Twob,1,2, and Author Three a

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## Guide to using this template on Overleaf

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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

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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.

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Please declare any conflict of interest here.

<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
1. 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.

cm wide. Use \begin{SCfigure\*}...\end{SCfigure\*} for a wide figure with side captions.

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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.

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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.

- 1. Belkin M, Niyoqi 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.

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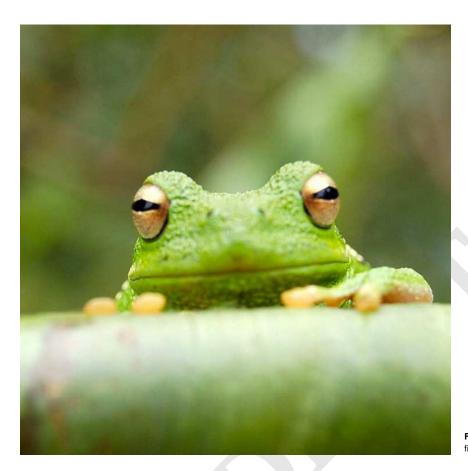
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**Fig. 2.** This caption would be placed at the side of the figure, rather than below it.

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

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

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