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This manuscript was compiled on February 9, 2023

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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
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.

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Subsection for Method. Example text for subsection.

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- 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.

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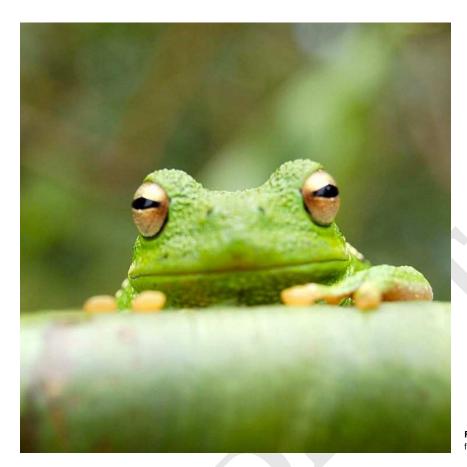
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**Fig. 2.** This caption would be placed at the side of the figure, rather than below it.

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

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

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

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