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

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

<sup>2</sup>To whom correspondence should be addressed. E-mail: [author.twoemail.com](mailto:author.twoemail.com)

the `\begin{figure*}...\end{figure*}` environment. Figures wider than one column should be sized to 11.4 cm or 17.8 cm wide.

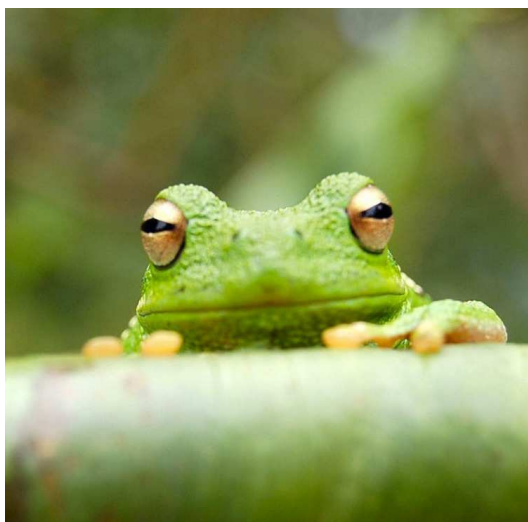
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$$\begin{aligned}(x + y)^3 &= (x + y)(x + y)^2 \\ &= (x + y)(x^2 + 2xy + y^2) \\ &= x^3 + 3x^2y + 3xy^2 + y^3.\end{aligned}\tag{1}$$



**Fig. 1.** Placeholder image of a frog with a long example caption 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.

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## 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 paper.

1. Belkin M, Niyogi P (2002) Using manifold structure for partially labeled classification in *Advances in neural information processing systems*. pp. 929–936.
2. Bérard P, Besson G, Gallot S (1994) Embedding riemannian manifolds by their heat kernel. *Geometric & Functional Analysis GAFA* 4(4):373–398.

**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.

3. 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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