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This manuscript was compiled on September 20, 2019

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## Guide to using this template on Overleaf

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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>&</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

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.

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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. M Belkin, P Niyogi, Using manifold stucture for partially labeled classification in Advances in neural information processing systems, pp. 929-936 (2002).
- 2. P Bérard, G Besson, S Gallot, Embedding riemannian manifolds by their heat kernel. Geom. & Funct. Analysis GAFA 4, 373-398 (1994).
- 3. RR Coifman, et al., Geometric diffusions as a tool for harmonic analysis and structure definition of data: Diffusion maps. Proc. Natl. Acad. Sci. United States Am. 102, 7426-7431 (2005).

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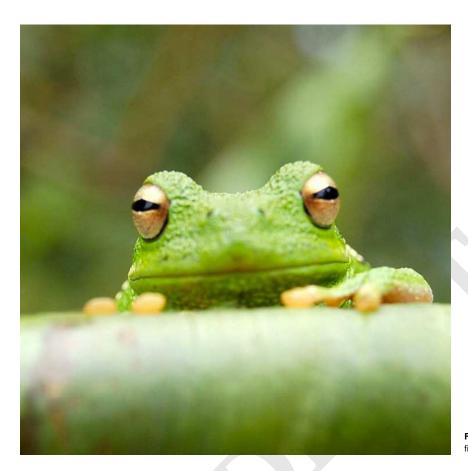
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**Fig. 2.** This caption would be placed at the side of the figure, rather than below it.

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

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

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

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