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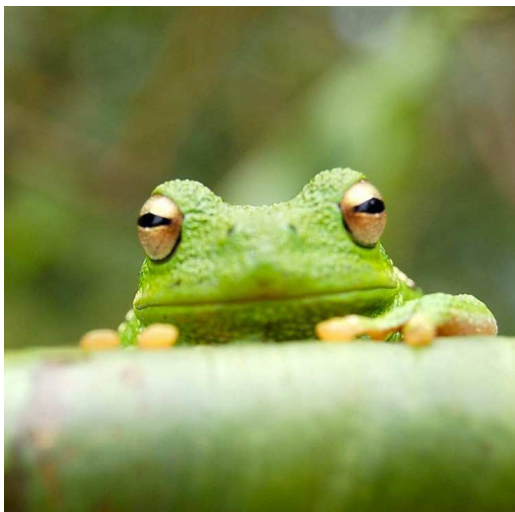
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Please declare any competing interests here.

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**Fig. 1.** Placeholder image of a frog with a long example legend 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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1. M Belkin, P Niyogi, Using manifold structure 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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## 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.

**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.

4. RJF Thomas, "Enamel defects, well-being and mortality in a medieval Danish village," PhD thesis, Pennsylvania State University, University Park, PA (2003).
5. TM Toolan, "Advances in Sliding Window Subspace Tracking," M.Sc. thesis, University of Rhode Island, Kingston, RI (2005).



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

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