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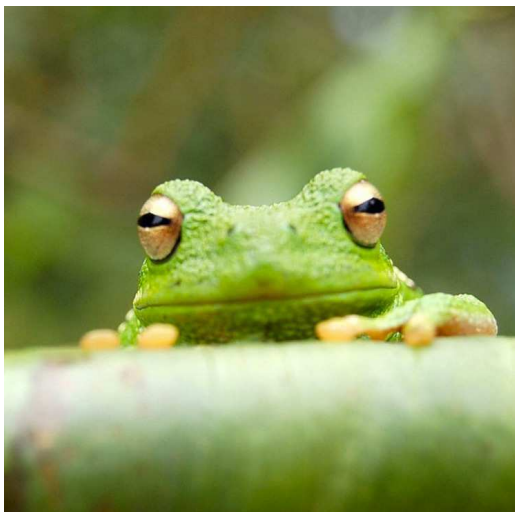
Fig. 1. Placeholder image of a frog with a long example legend to show justification setting.

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 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).

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

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Single column equations. Authors may use 1- or 2-column equations in their article, according to their preference.

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SI Appendix. Supply extended materials and methods information in a separate SI Appendix PDF file. Include SI movie legends. SI will be published as provided by the authors; it will not be edited or composed. Supplementary figures and tables are not allowed.

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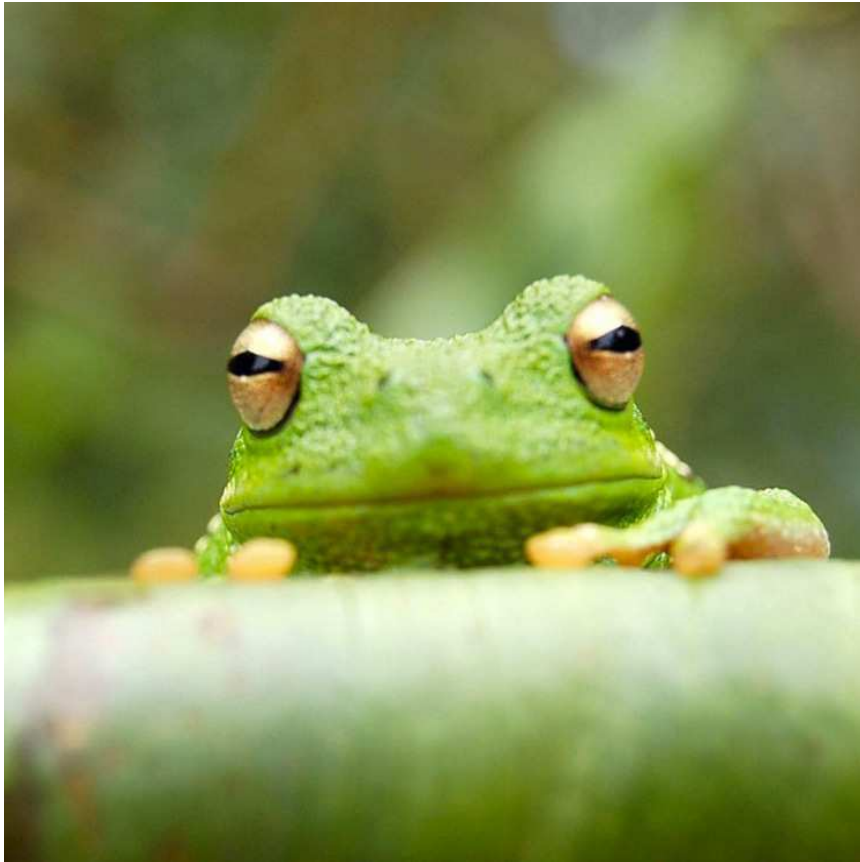
Materials and Methods

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.

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).

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

$$(x + y)^3 = (x + y)(x + y)^2$$
$$= (x + y)(x^2 + 2xy + y^2) \quad [1]$$
$$= x^3 + 3x^2y + 3xy^3 + x^3.$$