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¹A.O.(Author One) contributed equally to this work with A.T. (Author Two) (remove if not applicable).

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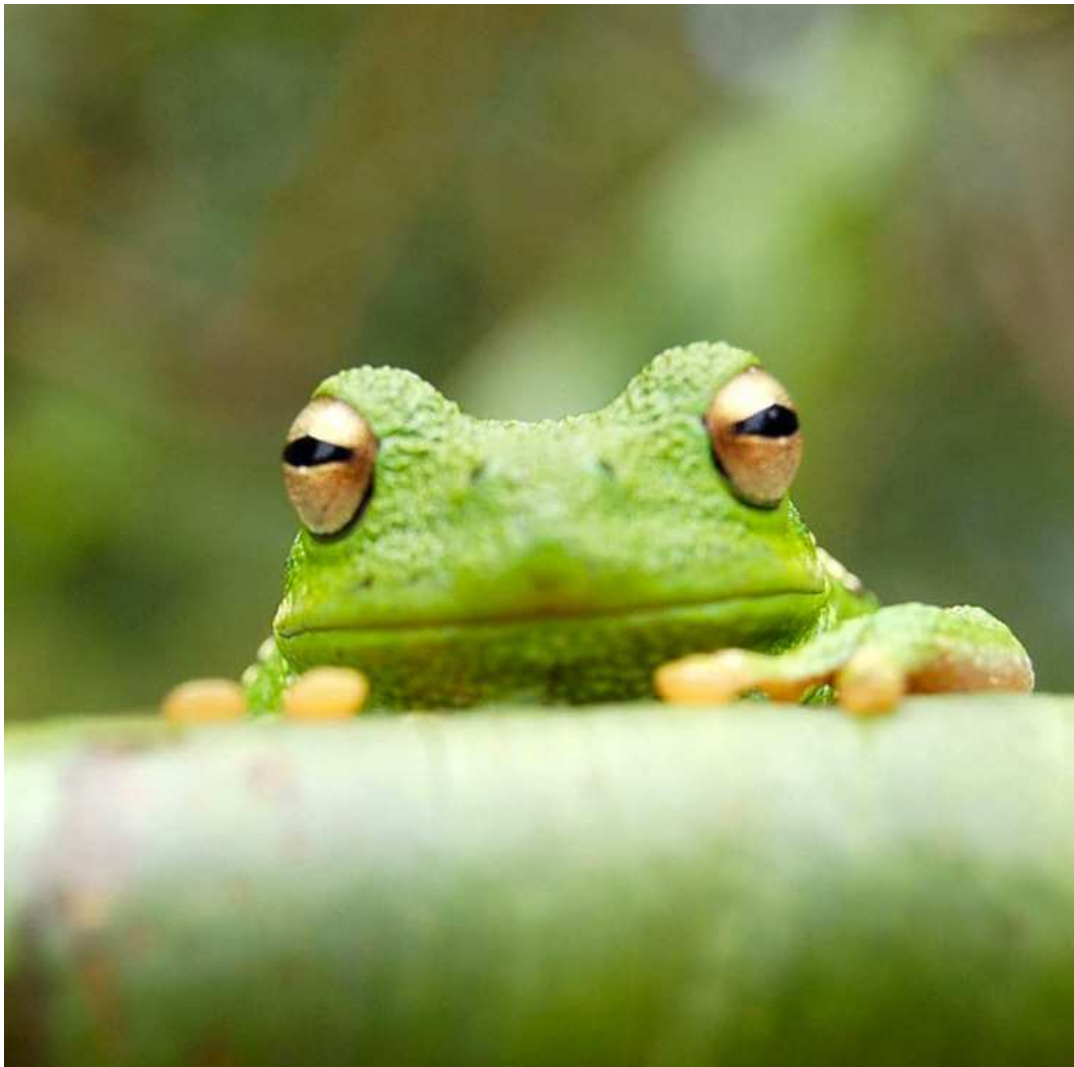


Fig. 1. Placeholder image of a frog with a long example legend to show justification setting.

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33 Images must be provided at final size, preferably 1 column width (8.7cm). Figures wider than 1 column should be sized to
34 11.4cm or 17.8cm wide. Numbers, letters, and symbols should be no smaller than 6 points (2mm) and no larger than 12 points
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39 Use `\begin{SCfigure*}... \end{SCfigure*}` for a wide figure with side legends.

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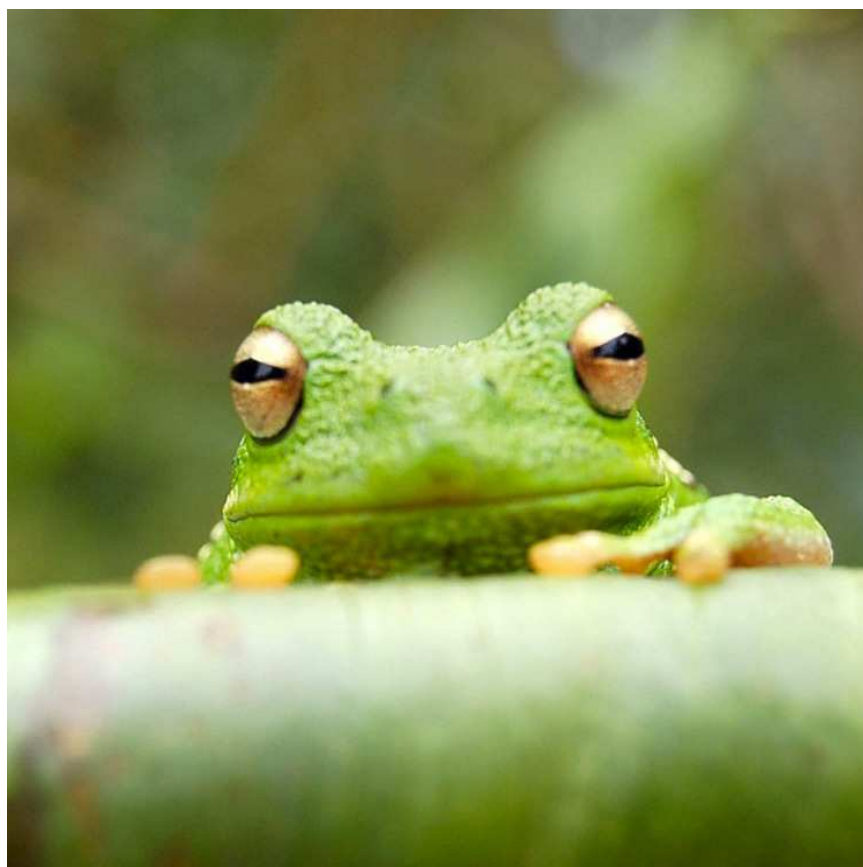


Fig. 2. This legend would be placed at the side of the figure, rather than below it.

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

42 To allow an equation to span both columns, use the `\begin{figure*}... \end{figure*}` environment mentioned above for
43 figures.

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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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59 **ACKNOWLEDGMENTS.** Please include your acknowledgments here, set in a single paragraph. Please do not include any acknowledgments
60 in the Supporting Information, or anywhere else in the manuscript.

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