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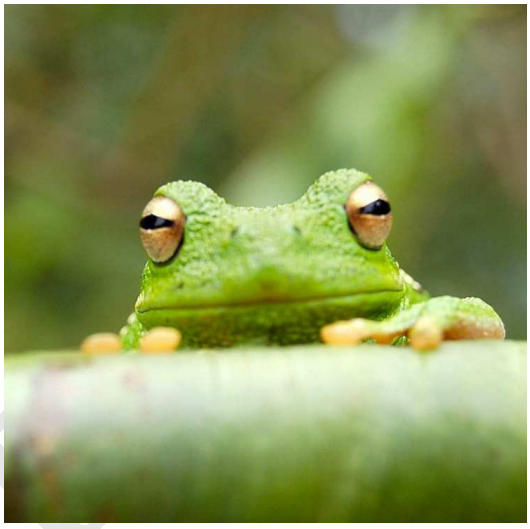

Fig. 1. Placeholder image of a frog with a long example caption to show justification setting.

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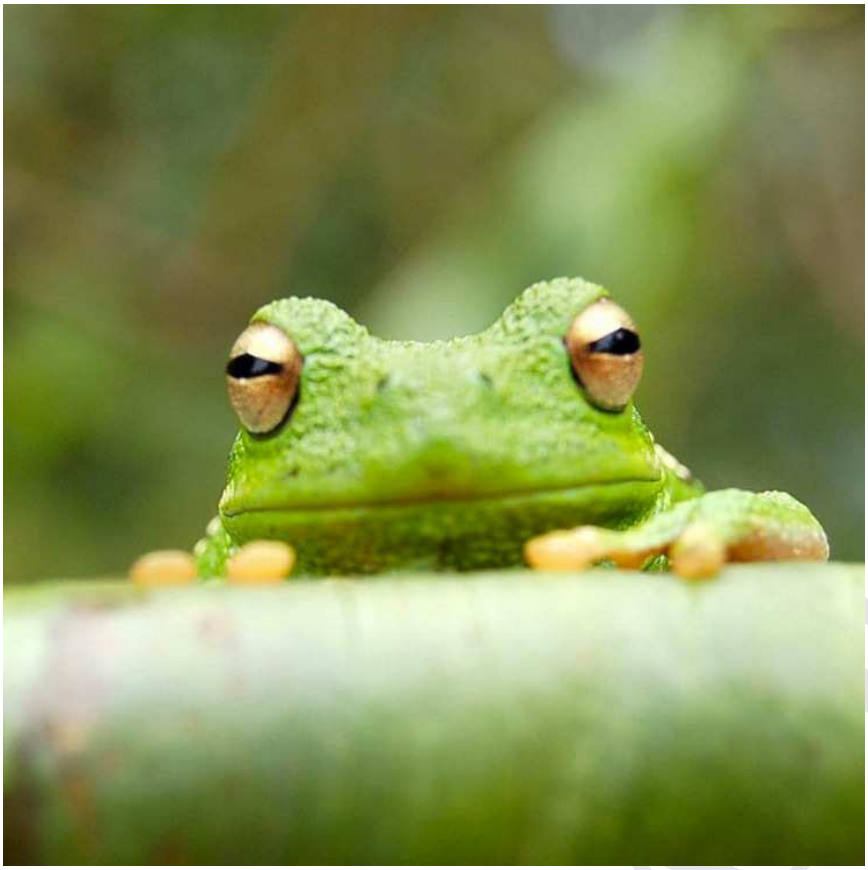

Fig. 2. This caption would be placed at the side of the figure, rather than below it.

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

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 captions.

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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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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. Belkin M, Niyogi P (2002) Using manifold stucture 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.
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.