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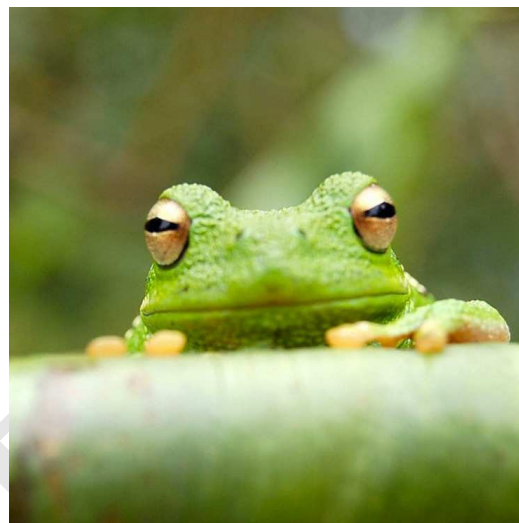


Fig. 1. Placeholder image of a frog with a long example caption to show justification setting.

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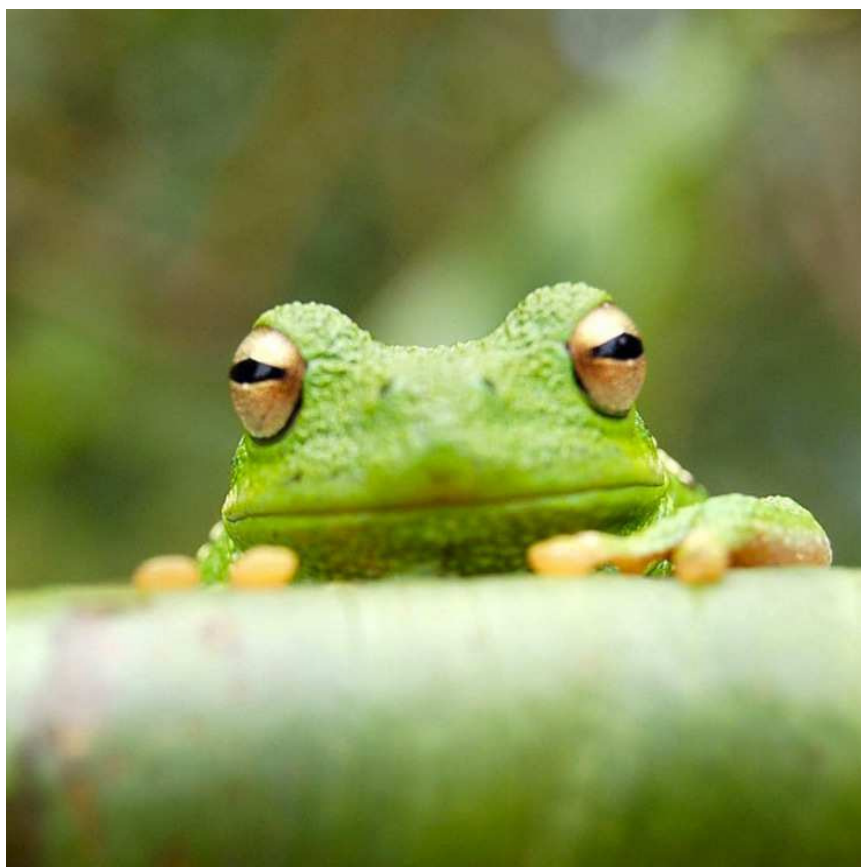
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Figure 1 shows an example of how to insert a column-wide figure. To insert a figure wider than one column, please use



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

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

68 the `\begin{figure*}... \end{figure*}` environment. Fig-  
 69 ures wider than one column should be sized to 11.4 cm or 17.8  
 70 cm wide. Use `\begin{SCfigure*}... \end{SCfigure*}` for a  
 71 wide figure with side captions.

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 87 ing types of SI: datasets, videos, and 3D figures. Extended  
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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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- 113 1. Belkin M, Niyogi P (2002) Using manifold structure for partially labeled classification in *Ad-*  
114 *vances in neural information processing systems*. pp. 929–936.
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116 *Geometric & Functional Analysis GAFA* 4(4):373–398.
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118 definition of data: Diffusion maps. *Proceedings of the National Academy of Sciences of the*  
119 *United States of America* 102(21):7426–7431.

DRAFT