

# PNAS Supporting Information Template

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## Supporting Information (SI)

The main text of the paper must stand on its own without the SI. Refer to SI in the manuscript at an appropriate point in the text. Identify each Supporting Information file. Each file type should be numbered beginning with 1 (e.g., Fig. S1 and Table S1). Authors are limited to no more than 10 SI files, not including movie files. Authors who place detailed materials and methods in SI must provide sufficient detail in the main text methods to enable a reader to follow the logic of the procedures and results and also must reference the online methods. If a paper is fundamentally a study of a new method or technique, then the methods must be described completely in the main text. Because PNAS edits SI and composes it into a single PDF, authors must provide the following file formats only.

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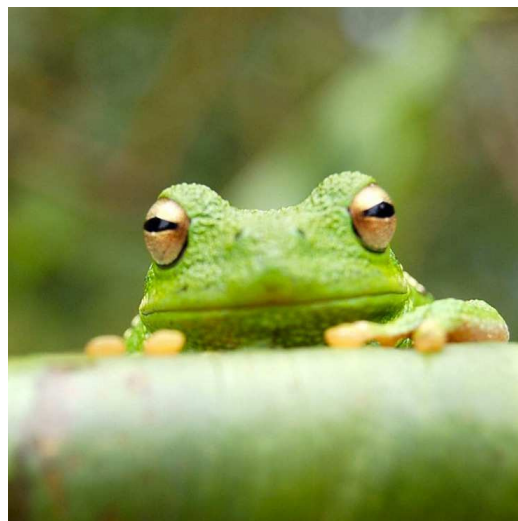
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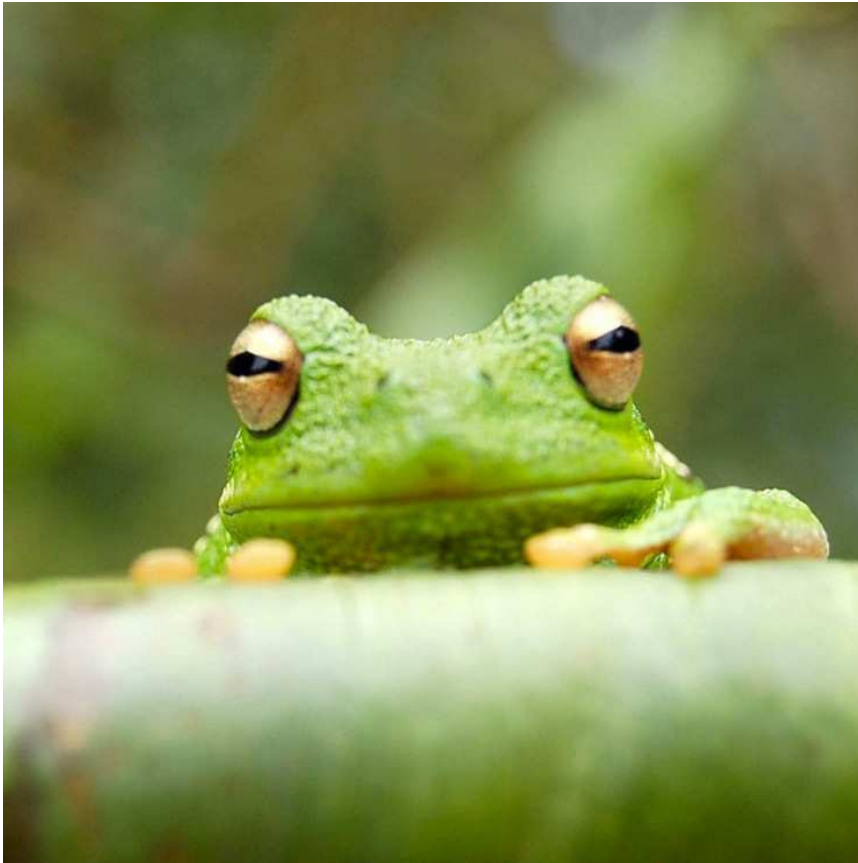


**Fig. S1.** Placeholder image of a frog with a long example caption to show justification setting.

**Table S1. 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.



**Fig. S2.** This caption would be placed at the side of the figure, rather than below it.

reproduction size and length. Movies should be no more than 10 MB in size.

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