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Gaussian09 NEB Program for Calculating Reaction Pathways[1]

JOHN-ERIC TIESSEN, Valparaiso University — The capability of calculating reaction pathways is an important aspect of modern materials chemistry and physics study. The goal of this work is to write a program to implement the Nudged Elastic Band (NEB) algorithm that can use the outputs of single point energy/force calculations from the electronic structure code of Gaussian09 to determine the reaction pathways, and activation energies, of chemical reactions. The NEB method is preferable to other minimum-energy-pathway searching methods in that it is more likely to find the most probable reaction pathway. The program aims to be well-documented easy to use, accurate, and efficient. Efforts are also made to make it easy to modify in the future for additional features. Testing cases, ranging from well documented chemical reactions to more complex systems, will be presented.

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