Gaussian09 NEB Program for Calculating Reaction Pathways

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.

1Special Thanks to: Professors Haiying He Stan Zygmunt