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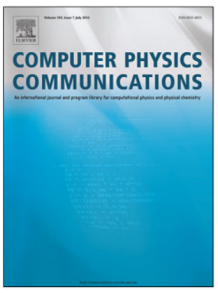

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PASTA: Python Algorithms for Searching Transition stAtes

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Abstract

Chemical reactions are often associated with an energy barrier along the reaction pathway which hinders the spontaneity of the reaction. Changing the energy barrier along the reaction pathway allows one to modulate the performance of a reaction. We present a module, Python Algorithms for Searching Transition stAtes (PASTA), to calculate the energy barrier and locate the transition state of a reaction efficiently. The module is written in python and can perform nudged elastic band, climbing image nudged elastic band and automated nudged elastic band calculations. These methods require the knowledge of the potential energy surface (and its gradient along some direction). This module is written such that it works in conjunction with density functional theory (DFT) codes to obtain this information. Presently it is interfaced with three well known DFT packages: Vienna Ab initio Simulation Package (VASP), Quantum Espresso and Spanish Initiative for Electronic Simulations with Thousands of Atoms (SIESTA). This module is easily extendable and can be interfaced with other DFT, force-field or empirical potential based codes. The uniqueness of the module lies in its user-friendliness. For users with limited computing resources, this module will be an effective tool as it allows to perform the calculations image by image. On the other hand, users with plentiful computing resources (such as

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