pysisyphus - Exploring Potential Energy Surfaces in Ground- and Excited States

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Abstract

Predicting the energetics of chemical transformations requires localizing stationary points on a potential energy surface. Whereas educts and products of a chemical reaction may be known, transition state optimization is challenging, as good guesses may be unavailable. Extending stationary point searches to excited states leads to additional difficulties as several states may be close in energy, requiring efficient state-tracking. Herein we report the implementation of pysisyphus, an external optimizer, that allows not only the localization of stationary points in the ground state, but also for excited states by providing several state-tracking algorithms. Pysisyphus offers all necessary tools for calculating reaction paths starting from the optimization of the reactants, running chain-of-states methods like the nudged elastic band or the growing string method with subsequent transition state optimization and a concluding intrinsic reaction coordinate calculation.

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