Accelerating Artificial Force Induced Reaction path search with Neural Network Potentials

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Kinetic studies provide mechanistic insights to understand and design novel chemical reactions. Unfortunately, constructing the reaction path network for a given system is a particularly challenging task. The Artificial Force Induced Reaction (AFIR) method provides an efficient framework for performing automated reaction path searches. However, these calculations typically incur high computational costs. Therefore, automated reaction path searches, at ab initio level, are restricted to relatively small systems or only considering reaction centers.

We propose to accelerate the AFIR-based reaction path search by replacing costly ab initio calculations with fast predictions from an adequately trained Neural Network Potential (NNP), which is the latest type of machine-learned force fields.

Unlike traditional application of NNP, we show that AFIR-based reaction path searches require especially robust models, which is particularly challenging for the current state of the art general-purpose NNP due to the lack of physics in their functional form.

To solve this challenge, we combined NNP models with a semi-empirical potential though **Δ**-learning. We found this combined model to be significantly more robust, while having an acceptable overall accuracy/cost balance.

We demonstrate, through practical examples, that our framework enables accurate reaction path searches at a reasonable cost on previously inaccessible systems.