PTPC2019

Contribution ID: **29** Type: **not specified**

Automated exploration of reactive potential energy surfaces

Friday, 11 January 2019 14:20 (25 minutes)

The determination of accurate rate coefficients remains a key challenge for a wide variety of chemical research areas, such as heterogeneous catalysis, liquid-phase chemistry and gas-phase processes. While research in the past decades has focused intensively on how to accurately calculate rate coefficients, the developed methods often incorporate several manual actions and need expert user knowledge. This is a particularly severe hinderance for finding reaction pathways, which forms the basis of rate coefficient calculations. Therefore, it is desirable to create tools that automatically search for reaction pathways, largely reducing the need for manual interventions. KinBot, our open-source code is one such tool, currently aiming at complex gas-phase chemical systems. It can uncover reaction pathways computationally in a way that is convenient for automated reaction mechanism generator and ab initio rate coefficient calculator codes, and can take advantage of high-performance computing facilities. KinBot aims to characterize all chemically significant stationary points on multidimensional potential energy surfaces as will be shown through various examples. A key step in finding reactions pathways is the ability to efficiently and robustly optimize to saddle points. Sella, our other open-source code achieves this goal via a series of algorithmic innovations demonstrated on literature benchmarks. Current research directions, such as the adaptation of our toolset to heterogeneous catalytic systems, will be also discussed.

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Session Classification: Reaction kinetics and mechanisms I