WestVirginiaUniversity®

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DEPARTMENT OF CHEMISTRY

Automated Chemical Kinetics

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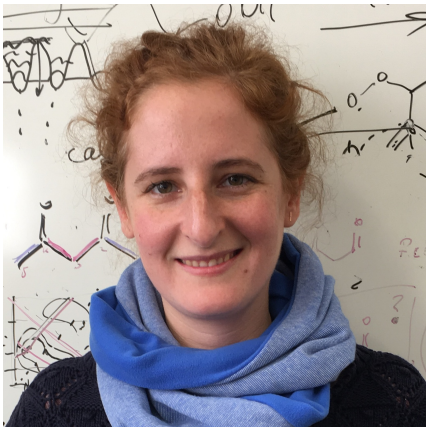

The determination of accurate rate coefficients remains a key challenge for a wide variety of chemical research areas, such as gas-phase processes, heterogeneous catalysis and liquid-phase chemistry. Research in the past decades has focused intensively on how to accurately calculate rate coefficients, but the developed methods often incorporate several manual actions and need expert user knowledge. This is a particularly severe hinderance for finding reaction pathways, which is the basis of rate coefficient calculations. It is, therefore, desirable to create tools that automatically search for reaction pathways, significantly reducing the need for manual interventions. KinBot, our open-source code, targets complex gas-phase chemistries, such as the ones found in combustion and atmospheric reaction systems. KinBot 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 is designed to find and characterize all chemically significant stationary points on multidimensional and multiwell potential energy surfaces - as we will demonstrate in several examples. In a separate effort we are developing a computational tool to uncover reaction pathways in heterogeneous chemistry, currently pursuing relatively simple reactions of small molecules and radicals on various metal facets

Students, meet the speaker after the seminar in a student/postdoc session from 5:45-6:15 pm

Date: Wed, Oct. 14, 2020
Time: 4:30-5:30 pm
Location: Virtual Seminar (Zoom)

https://wvu.zoom.us/j/91308678279?pwd=dU1EZEF6bm1FNVhyVDQ0OGNleGcwQT09