

## KinBot: An Automated Tool to Explore Elementary Reactions

Optimization of new transportation fuels and engine technologies requires characterization of the combustion chemistry of a wide range of fuel classes. Theoretical studies of *elementary* reactions — the building blocks of *complex* reaction mechanisms —, are essential to accurately predict important combustion processes such as autoignition of biofuels. The current bottleneck for these calculations is a user-intensive exploration of the underlying potential energy surface (PES), which relies on the “chemical intuition” of the scientist to propose initial guesses for the relevant chemical configurations. For newly emerging fuels, this approach cripples the rate of progress because of the system size.

In this poster, we present the current stage of the KinBot code, which we develop in order to automate the exploration of PES's. We present our current and planned strategies, as well as illustrate the capabilities of the code.

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