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Laboratory:PC2A

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Eventually,

CaPPA Work Package: WP-1 From gas phase to aerosols (for example)

# Theoretical investigation of the combustion kinetics of potential biofuels

To reduce fuel consumption, Greenhouse Gases, $NO_x$ and soot particles emissions, recent developments in engine technology have focused on operating internal combustion engines at **lower temperatures** and **fuel concentrations**. These constraints have motivated the apparition of Exhaust Gas Recirculation (EGR) technology, and triggered interest in Low-Temperature Combustion (LTC) engines. In these conditions, combustion chemistry is more complex as it relies on the formation of peroxides. Chemical branching is degenerate and highly **fuel-specific**. To accommodate the use of modern fuels such as biodiesels or fuels produced from biomass, **predictive models** of this combustion chemistry must be constructed and validated.

Recently, the interest has grown on the use of liquid fuels produced from lignocellulosic biomass. Because of the presence of **heteroatoms** (O, N) in their chemical structure, specific reaction pathways can be observed, rendering the utilization of typical rate rules for the prediction of rate coefficients difficult. However, **dedicated tools** for the exploration of **potential energy surfaces**, such as Kinbot, have been developed. This tool allows the automation of the calculation of the transition states and products for a given reactive system. The purpose of this work will be the implementation of the **Kinbot** code on the University's HPC cluster, and its use to investigate the complex reactive systems relative to novel biofuels. Specifically identified rate constants will be determined with help from **quantum chemistry calculations at a high level of theory**.

Keywords: Pollutant reduction, combustion, kinetic modeling, ab initio