

Seminar

First-principles investigation of stereo-electronic factors governing elementary steps of low-temperature hydrocarbon combustion

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Low-temperature hydrocarbon combustion (LTC) is a promising approach to reduce emissions, improve fuel efficiency, and enhance engine performance compared to high-temperature combustion. The reaction mechanism of low-temperature combustion involves a complex series of reactions between closed-shell and open-shell hydrocarbon species with molecular oxygen, leading to several reaction intermediates. Experimental observation of these intermediates is essential to establish the reaction mechanism. However, these intermediates are elusive due to their short lifetime. In 2015, Savee et al successfully detected one such radical, QOOH, through molecular design. This presentation will focus on the effect of stereo-electronic factors on the stability of these intermediates, providing design principles for future synthetic efforts to identify systems with desirable properties for low-temperature combustion. Accurate estimation of the thermochemical properties of all possible species is crucial for identifying these design principles. We will discuss how the W1 ab initio method is used to obtain high-fidelity thermochemical properties for elementary reactions involved in the low-temperature combustion of alkyl radicals. Additionally, we will explore the possibility of lowering the computational cost by using appropriate density functional theory while maintaining the accuracy of the results. We will also explore mechanistic details of the unimolecular dissociation path of QOOH using reaction force constant analysis.

Tuesday, Nov 26th 2024

11:30 Hrs (Tea / Coffee 11:15 Hrs)

Auditorium, TIFR-H