Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Students' Annual Webinar

Accurate thermochemical data and DFT benchmarking for elementary reactions in combustion chemistry

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Combustion engines, the key ingredient behind the majority of the world's energy production endeavours, are driven by low-temperature hydrocarbon oxidation. The process involves a series of reactions between closed-shell and open-shell hydrocarbon species with molecular oxygen that follows the low-energy pathway out of myriad possibilities. Identifying fuels with desirable properties, therefore, requires a highly accurate estimation of thermochemical properties of all possible species and subsequently determining the most favourable pathway. Because of its favourable cost and high accuracy, composite ab initio methods are desirable for in silico modelling of these species. In this talk, we will discuss how one such ab initio method, W1U, is used to obtain high-fidelity thermochemical properties for elementary reactions involved in the low-temperature combustion of alkyl radicals. Further, we will investigate if the computational cost can be lowered by using a suitable density functional theory while preserving accuracy.

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9:30 AM