Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Internal Seminar

High-throughput modeling of auto-ignition reaction pathways across the chemical space of hydrocarbons

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Organic oxidation reactions in processes such as auto-ignition and tropospheric reactions proceed through the peroxy (ROO) and hydroperoxyalkyl (QOOH) radicals. The stability of these radicals govern the efficiency of radical propagation chain reactions. In particular, QOOH upon unimolecular decomposition, or via subsequent bonding to O_2, yields highly reactive OH radicals, thereby sustaining the essential steps leading to ignition. In the troposphere, isomerization of ROO to QOOH is also observed. While the importance of these intermediates has been reported, QOOH has been elusive to experimental detection. This motivates us to explore the chemical space of the radicals/molecules in this specific reaction scheme.

We seek to identify all possible ROO, QOOH radicals that can be generated from a set of 4890 hydrocarbons that are subset of the 134kilo dataset [1] and combinatorially explore all possible reaction pathways that these radicals undergo involving collectively over 4.5 Million ROO/QOOH/OOQOOH radicals, cyclic ethers and alkenes. Challenges arising in the automation of the calculations, preliminary results and future plans to host this dataset on the MolDis platform [2] will be discussed.

References:

[1] Quantum chemistry structures and properties of 134 kilo molecules, R. Ramakrishnan, P.O. Dral, M. Rupp, O.A. Von Lilienfeld, Scientific data 1, 140022, 2014.\\
[2] https://moldis.tifrh.res.in/

Monday, Apr 29th 2019

1:30 PM (Tea/Coffee at 1:15 PM)

Seminar Hall, TIFR-H