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

Seminar

Probing and tuning the chemical reactions at a single molecular level

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The traditional chemical analysis techniques for probing the reaction kinetics, such as Mass spectrometry, NMR, IR, and UV-Vis spectroscopy, have certain detection limits associated with them (i.e. in the order of few ppm). It is not trivial to further increase the detection limit of these traditional techniques to a single molecule level. In this context, we envisage that the highly sensitive MCBJ technique can become a promising platform for reaction detection studies with the lowest detection boundary, i.e., single-molecule level. To achieve this goal, two immediate strategies one had to develop were finding a way to carry out the reaction within the MCBJ setup and correlating the data (conductance-distance traces) collected corresponding to the molecular junction to the in-situ chemical reaction. The conductance-distance traces obtained after the measurement serve as a fingerprint for the molecular system under observation, and the continuous measurement of conductance-distance traces of the molecular junction throughout the chemical reaction serves as a matrix to extract the rate information. Then, the precise data analysis methodology was developed for getting the presence and proportion of different molecular species (reactant/product/intermediate) inside the reaction mixture from the bulk data using machine learning tools. Using this framework, we have tried to probe various chemical reactions at a single molecular level. In my talk, I will give a brief overview of different chemical reactions that we are probing at single molecular level.

Wednesday, Nov 8th 2023

4:00 PM (Tea / Coffee 3.45 PM)

Auditorium, TIFR-H