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

Seminar

Quantum chemical explorations across diverse chemical spaces

Sabyasachi Chakraborty

TCIS, Hyderabad

The discovery of functional molecules requires investigations into hitherto unknown regions of the chemical universe. While this space may seem infinite, agreeing upon the specific constitution and structural features allows us to limit our search space to a finite set. Enumeration provides an exact count of the entries for an exhaustive generation. However, the sheer size often rules out any synthesis endeavors and forces us to adopt a virtual realisation. Fortunately, advances in computational technology and accurate quantum theories over the past few decades have led us to traverse these spaces in a high-throughput fashion and identify transferable chemical trends that may guide specific synthesis endeavors. In this talk, we will highlight the significance of chemical space design and discuss the diverse techniques employed to address the spaces explored here. We will identify novel chemical trends from molecular properties obtained in a high-throughput fashion via ab initio modelling and comment on the scope of different machine learning protocols as surrogates to such expensive calculations. We will also discuss the need for reliable computational workflows for high-throughput explorations. Furthermore, we will demonstrate how chemical space design allows us to improve the existing theoretical protocols and discuss a novel theoretical scheme to calculate ion-pair interaction energies in biomolecules.

Thursday, Jul 14th 2022

04:00 PM (Tea/Coffee at 3:45 PM)

Auditorium, TIFR-H