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

# Students' Annual Seminar

## Non-covalent interactions across chemical datasets using Symmetry Adapted Perturbation Theory (SAPT)

## Sabyasachi Chakraborty

Understanding non-covalent interactions across chemical space are important to design molecular materials with desirable stability and optoelectronic activity. Symmetry Adapted Perturbation Theory (SAPT) describes the various components of non-covalent interactions between dimers as physically meaningful quantities and provides quantitative accuracy for long-range interactions (3-20 Ang.) thus, justifying its use for such endeavours.

As a first step in designing optoelectronically active, heteroatom substituted organic crystals/composite systems, we have enumerated the complete chemical space of B, N - substituted polycyclic aromatic hydrocarbons and discovered molecules with desirable electronic properties.

A long-standing problem that has eluded critical analysis is the first-principles quantification of the components of salt-bridge interactions in bio-molecules. To this end, we have applied Intramolecular SAPT (ISAPT) – a variant of SAPT for intramolecular interactions – on model peptides and analysed mid-range (2-3 Ang.) interactions in detail. To validate ISAPT for mid-range problems we have devised a thermodynamic cycle. The relevance of the SAPT Ansatz, in general, to strongly coupled interactions will be discussed. The talk will also highlight method development studies planned to widen the scope of SAPT to mid-range, partially covalent problems.

***Friday, Apr 26th 2019***

***10:00 AM (Tea/Coffee at 9:30 AM)***

***Seminar Hall, TIFR-H***