Studying chemical reactions using transition state modeling

Our research focuses on chemical reactivity and catalysis. When two molecules react to form product(s), there are different likely pathways that one can think of. Energies of various intermediates and transition states connecting such intermediates involved in the reaction has an enormous effect on the pathway a reaction would proceed through. We employ *ab initio* and density functional theory computational methods to identify the nature of intermediates and transition states involved in catalytic reactions. Aided by the knowledge of the structure and energetics of a given reaction, we design new variations of catalysts. Computational design of catalysts is an emerging domain of research where first principles computations help us arrive at potentially leads for new catalysts.

Considering that a large number of compounds used as prescription drugs are chiral, there is an ever-increasing requirement for more efficient methods for the generation of chiral molecules. Another area of our expertise is in asymmetric catalysis, which is a process wherein one enantiomer is selectively produced. The control of enantiomeric composition in a reaction is directly related to the transition state energies. Our objective is to gain insights into the energetic features of the transition states and thereby suggest rational modifications for improved processes in asymmetric catalysis.

Prof. R. Sunoj, Department of Chemistry, sunoj@chem.iitb.ac.in