Understanding the micro-level energetics and dynamics of non-covalent interactions between organic systems and solvents

Renjith Thomas

Department of Chemistry, St Berchmans College (Autonomous), Mahatma Gandhi University, Changanassery 686101, Kerala INDIA

renjith@sbcollege.ac.in

ABSTRACT

Non-covalent interactions are crucial forces that hold molecules or molecular complexes together without forming chemical bonds. These interactions include van der Waals forces, hydrogen bonding, electrostatic interactions, and hydrophobic effects. They play pivotal roles in the structure and function of biological molecules like proteins, DNA, and RNA and are central to many biological processes. One key aspect of non-covalent interactions is their role in solvation, which dictates solute-solvent interactions' strength and specificity. For instance, hydrogen bonds may stabilize a hydration shell around a solute, while van der Waals forces and hydrophobic effects can promote the aggregation of non-polar solute molecules in a solvent.

The application of computational tools, such as the Non-Covalent Interaction (NCI) method developed by Yang and colleagues, allows for detailed visualization and analysis of these interactions within chemical systems. This method utilizes the reduced density gradient (RDG) and electron density metrics to identify and characterize the regions of weak interactions crucial for biological functions. The NCI approach, along with techniques from Atoms In Molecule (AIM) theory by Bader, which uses electron density to define molecular boundaries and interactions, provide powerful ways to predict and manipulate these interactions for better understanding of solvation dynamics and interaction mechanisms.

This lecture aims to go into the diverse non-covalent interactions between biomolecules and solvents, emphasizing how computational chemistry tools can be harnessed to explore these interactions.

Reference

Jisha Mary Thomas and Renjith Thomas, Study of Non-Covalent Interactions Present in the Tapinarof–Ethanol System with Special Emphasis on Hydrogen-Bonding Interactions J. Phys. Chem. B 2023, 127, 26, 5933–5940