Understanding Intermolecular Interactions: Computations on Complex Systems

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Weak intermolecular forces like H-bonding and π-stacking are central to processes at the biological as well as material sciences. The relatively lesser penalty associated with breaking such weak interactions allow the molecules to dynamically transform between various states of aggregations. This leads to exotic properties like polymorphism and molecular bistability. From a computational viewpoint, such systems bring immense challenge due to the lack of realistically affordable methods within conventional wavefunction based descriptors on one hand and the lack of proper dispersion corrections within the popular density functional (DFT) formalism on the other. Therefore, modeling such interactions requires a non-trivial and out-of-the black box solutions. The talk will focus on two separate examples: (1) a molecular rotor and (2) multi-centered π-stacked magnetic interactions, wherein we have modeled such weak intermolecular interactions. The computed results are compared with experimental data to justify the suitability of our approach.