Abstract for Ph.D. Open Seminar
Department of Chemistry, IISER Bhopal

Title of Seminar: Unravelling the Role of Polymorphism and Interaction Topology towards a Quantitative Assessment of Intermolecular Interactions in Molecular Crystals.

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Time: 11.00am **Venue**: AB2-401

The understanding of the crucial role of different competitive and cooperative intermolecular interactions in promoting the structural diversity in crystalline solids is a key attraction in supramolecular chemistry.[1,2]In particular, the occurrence of multiple crystalline phases of any given molecule (polymorphs), including crystallization with guest solvent molecules (solvates), having distinct physicochemical and material properties, provide great opportunities to tune the structure−function relationships at the molecular level.[3]

The extensive crystallization screening in a library of small molecules containing halogenated*N*-ethynylphenylbenamides has resulted in the formation of different crystal polymorphs, andsolvates of the unique guest hexafluorobenzene.In the current work, the dynamic nature of crystal polymorphism was evaluated in terms of *single-crystal-to-single-crystal* polymorphic phase transition induced by hydrophobic silicone oil[4] and rapid desolvation of the guest solvent hexafluorobenzene[5] in various fluoro-substituted compounds. The inclusion chemistryof various substituted *N*-ethynylphenylbenamides host was also explored based on the features of host−guest stacking interactions.[6]Furthermore, nanoindentation study was performed to understand the role of structureon the observed mechanical properties (hardness and elastic modulus) in the crystalline polymorphs of *meta*-fluorinated *N*-ethynylphenylbenamide[7] and the solvates of twobiologically promising dihydropyrimidine analogues.[8]

Finally, the obtained crystal structure landscape of the unsubstituted molecule, namely, *N*-ethynylphenylbenamide, was experimentally mapped through the method of chemical modification of the parent compound and the device of polymorph formation.[9]The solid-state structural landscape was further investigated with inputs from the quantitative analysis of the interaction topological landscape via the approach of energy frameworks[10],which was also validated through the method of crystal structure prediction.

References

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