S N BOSE NATIONAL CENTRE
FOR BASIC SCIENCES
Block JD, Sector III, Salt Lake, Kolkata 700 106

DEPARTMENTAL SEMINAR

Chemical and Biological Sciences

21st April 2026 **4.00 PM** **ONLINE / FERMION**

SPEAKER

Dr. Deepak Chopra,
Professor, Department of Chemistry,
Indian Institute of Science Education and Research, Bhopal

TITLE OF THE TALK

Understanding the Role of Weak Intermolecular Interactions involving Organic Fluorine: Insights from Quantum Crystallography

ABSTRACT

The prevalence of non covalent interactions is central to chemistry and biology [1]. Conventional H-bonds are well understood [1] but the role of weak intermolecular interactions, particularly those involving organic fluorine, in the formation of weak H-bonds has been questioned [2]. It was initially envisioned that such weak contacts would evolve only in the absence of strong H-bonds [3]. Detailed investigations, in the past two decades, from high resolution charge density and QTAIM analysis, into the electronic features of fluorine based contacts have established the role of weak C-H…F-C contacts in polymorphs [4]. Furthermore, the importance of C-F…F-C [5] and C-F…O [6-7] contacts in the solid state have also been realized. Interestingly some of these contacts were observed in in situ cryocrystallized liquids [5-6]. It has been observed, that the existence of interactions involving organic fluorine are not a consequence of crystal packing and have implications in the events of molecular recognition in the solid state. Furthermore, the role of fluorine as a halogen bond donor has also been investigated in detail using different computational approaches as well [7]. All these studies explore the applications of quantum crystallography to unravel the importance of weak interactions involving fluorine in crystalline solids.

References:
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HOST FACULTY

Prof. Suman Chakrabarty, Professor

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