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

Title of Seminar: Investigation on Magnetic Bistable Systems, Fe(III) Based Spin Crossover (SCO) and Cu-Ln Coupled Single-Molecule Magnet (SMM).

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Time: 4 p.m.

Thesis Supervisor: Dr. Sanjit Konar

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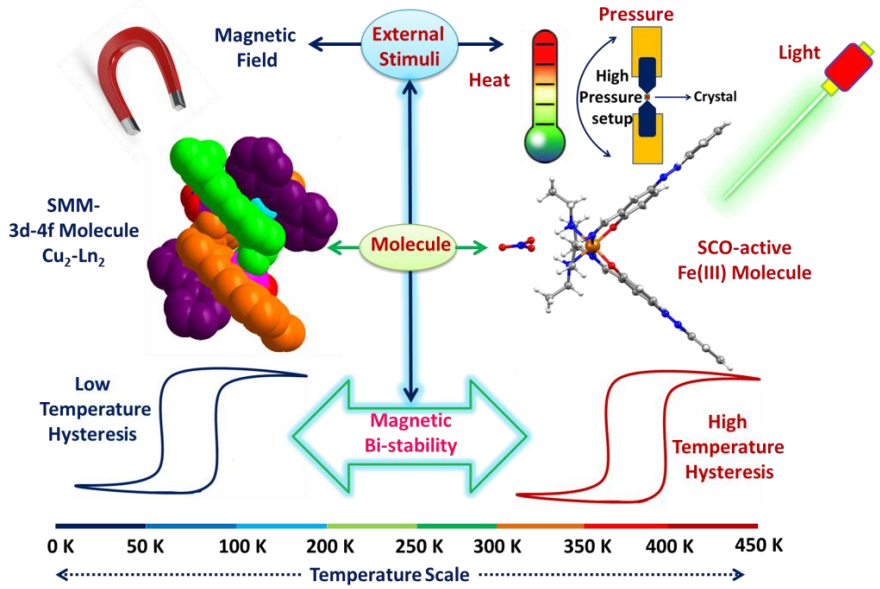
Venue: AB2-401

Abstract: In the current world of digitization data plays an important role in every aspect of our daily lives. Data is stored by magnetizing and demagnetizing some magnetic bistable materials, where each state corresponds to a digit of information.[1] For this reason, magnetic bistable molecules are an interesting field of research.[2] In these molecules, it may be possible to store information as a magnetic response by the help of external stimuli such as heat, light, magnetic field, and pressure.[3] Two major magnetic bistable systems are single-molecule magnet (SMM)[4] and spin crossover (SCO).[5] SMMs operate at a lower temperature while SCO can operate at room temperature and above (Scheme 1).

My doctoral thesis focuses on these two aspects, SMM for Cu-Ln pair and SCO for Fe(III) systems. For SMM, we have synthesized Cu-Ln coupled molecules using a mixed ligand (H_4L^1, H_2L^2) and mixed metal strategy (Cu and Ln = Dy, Gd, Tb) for the preparation of magnetic refrigerant (Cu_2-Gd_2) and SMMs (Cu_2-Dy_2, Cu_2-Tb_2).[6] In the mixed ligand systems, a flexible dihydrazide based oxygen donor rich ligand (H_4L^1) is used which can easily bind with lanthanides (Ln) along with a tridentate ligand (H_2L^2) which can coordinate with transition metal



Scheme 1. Schematic representation of SMM (low-temperature region) and SCO (high-temperature region) molecules with their respective external stimuli required for their function.

(Cu) easily. Also by increasing the flexibility of the ligand, nuclearity of the Cu-Ln complexes also increased. Control on the nuclearity of these multi-nuclear (Cu_2Ln_4 and Cu_4Ln_4, Ln = Dy, Gd)[7] complexes was achieved by varying reaction conditions.

For investigation on SCO, we have addressed a new perspective of designing SCO molecules with azo-phenyl substituted ligand that can respond to light, making them suitable candidates for photo-magnetic materials.[8] In a separate attempt we tried to rationalize the role of ligand field strength on SCO process by the use of three complexes whose only difference is the substituents, [Fe(5-X-SalEen)$_2$]NCS; X = Me (**1**), X = Br (**2**), X = OMe (**3**). These complexes have been synthesized and analyzed experimentally as well as theoretically.[9] This understanding can be useful for rationalizing the synthesis of SCO molecules. Also, a set of three complexes [Fe(X-OMe-SalEen)$_2$]NCS·nH_2O; X = 3-OMe, n = 0 (**1**), 4-OMe, n = 1.5 H_2O (**2**), 5-OMe, n = H_2O (**3**) have been synthesized and investigated to understand how the same substituent can affect SCO process from a different isomeric position (ortho, meta, and para-substituted) of a phenyl ring.[10]

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