IIT Kharagpur PLATINUM JUBILEE

S. N. BOSE NATIONAL CENTRE FOR BASIC SCIENCES

4th International Conference on
SPINS IN MOLECULAR SYSTEMS (SIMS) 2025

Jointly organised by IIT Kharagpur and SNBNCBS Kolkata

29th November - 01st December, 2025

Book of Abstracts

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Message from Director, Indian Institute of Technology Kharagpur

It gives me great pleasure to extend my warm greetings to all the participants of the International Conference on "**Spins in Molecular Systems (SIMS 2025)**", jointly organized by the Indian Institute of Technology Kharagpur and the S. N. Bose National Centre for Basic Sciences, Kolkata, during November 29 – December 1, 2025.

This conference marks the fourth edition of a highly successful international series that began at the Indian Institute of Science, Bangalore, and has quickly established itself as a leading platform for discussion and collaboration in the field of molecular spin science. I am delighted that IIT Kharagpur, in association with S. N. Bose Centre, is hosting this edition and carrying forward this important scientific tradition.

The study of spins in molecular systems lies at the confluence of chemistry, physics, and materials science, and has profound implications for quantum technologies, spintronics, and molecular electronics. By bringing together distinguished researchers, young scientists, and students from across the world, SIMS 2025 will provide a vibrant forum to exchange ideas, present recent findings, and explore new frontiers in this rapidly evolving area.

I am confident that the discussions and interactions during this conference will inspire new collaborations and stimulate innovative approaches to some of the most pressing challenges in modern molecular science.

I take this opportunity to congratulate the organizers for their dedicated efforts in putting together such a timely and significant event, and I wish SIMS 2025 great success. May this conference serve as a catalyst for advancing fundamental understanding and fostering the next generation of scientific breakthroughs in molecular spin systems.

Suman Chakraborty

Prof. Suman Chakraborty
Director
Indian Institute of Technology Kharagpur

Message from Director, S. N. Bose National Centre for Basic Sciences Kolkata

I feel extremely happy that the international conference "Spins in Molecular Systems 2025 (SiMS 2025) is being jointly organized by IIT Kharagpur and SNBNCBS Kolkata. I must congratulate the organizers for putting together a fantastic programme with excellent speakers. The choice of topics which ranges from fundamental science like Molecular Spin Crossover and Spin-State Switching to emerging applications is praiseworthy. I am sure this conference will serve as a learning experience for young students and a great networking platform to senior colleagues. I wish all the success of the conference.

Prof. Tanusri Saha-Dasgupta
Director
S. N. Bose National Centre for Basic Sciences, Kolkata

4th International Conference on

Spins in Molecular Systems (SIMS) 2025

Jointly Organised by IIT Kharagpur and SNBNCBS Kolkata

November 29 - December 01, 2025

Venue: IIT Khagarpur Research Park, Kolkata

Day 1 (November 29, 2025) Saturday
Venue: Research Park Auditorium (Ground Floor)

08.00 - 09.15	Registration at the Venue
09.15 - 10.00	Inauguration
Session - 01 (Chair: Anjan Barman, SN Bose National Centre, India)	
10.00 - 10.25	**Masahiro Yamashita, Tohoku University, Japan** Molecular Spin Qubits toward Quantum Computer Based on Cu(II), Ni(III), Co(II), Fe(III), Mn(II), Cr(V), and V(IV) Complexes with S = 1/2
10.25 - 10.50	**Ramaswamy Murugavel, IIT Bombay, India** Single Ion Magnetism in Lanthanide Organophosphates and Phosphonamides
10.50 - 11.15	**Bolvin Hélène, Université Paul Sabatier, France** Probing the magnetic properties of actinide complexes by paramagnetic NMR
11.15 - 11.45	Tea-Break
Session - 02 (Chair: Pradip Pachfule, SN Bose National Centre, India)	
11.45 - 12.10	**Talal Mallah, Université Paris-Saclay, France** Ni(II) Complexes as Electronic Spin Qubits with a Clock Transition
12.10 - 12.35	**Sreetosh Goswami, IISc Bangalore, India** Molecular Neuromorphic Building Blocks for Artificial Intelligence
12.35 - 13.00	**Sanjit Konar, IISER Bhopal, India** Stimuli Responsive Magnetic Molecules
13.00 - 13.25	**Sabyasachi Roychowdhury, BITS Pilani, Dubai** Probing the Reliability of Structural Hallmarks in Uranium-Soft Ligand Interactions
13.25 - 13.40	Technical Talk: Rigaku
13.40 - 16.00	Conference Picture I, Lunch and **Poster Session - I (9th Floor Cafeteria)**
Session - 03 (Chair: Arghya Taraphder, IIT Kharagpur)	
16.00 - 16.25	**S Ramasesha, IISc Bangalore, India** Modeling Blocking Temperature by Kinetic Monte Carlo Method
16.25 -16.50	**D. D. Sarma, IISc Bangalore** In search of 1-dimensional systems, hosting quantum spin liquids
16.50 - 17.15	**Swapan K Pati, JNCASR Bangalore, India** Understanding the Quantum Entangled Phases and Quantum Spin Liquid Candidates through Multiscale Modeling
17.15 - 17.40	Tea-Break

Session - 04 (Chair: Sanjoy Bandyopadhyay, IIT Kharagpur)	
17.40 - 18.00	**Mousumi Das, IISER Kolkata** Role of Spin Multiplicity of Molecular Excited States in Designing Photovoltaics and TADF Materials
18.00 - 18.20	**Rajamani Raghunathan, UGC-DAE Consortium, India** Spin Polarised Antiferromagnets
18.20 - 18.40	**Geetanjali Giri, VIT Bhopal, India** Electronic Structure and Spin Dynamics in Multiferroics
18.40 - 19.10	Felicitation of S Ramasesha on his 75th Birthday (Chair: Varadharajan Srinivasan, IISER Bhopal, India)
19.30 - 22.30	Cake Cutting and Dinner
Day 2 (November 30, 2025) Sunday **Venue: Research Park Lecture Hall (7th Floor)**	
Session - 05 (Chair: Masahiro Yamashita, Tohoku University, Japan)	
09.30 - 09.45	Rigaku International Award Announcement
09.45 - 10.10	**Partha Sarathi Mukherjee, IISc Bangalore, India** (Rigaku International Award Lecture) Chemical Transformations in Molecular Flasks
10.10 - 10.35	**Shinya Hayami, Kumamoto University, Japan** Slow Magnetic Relaxation in Spin Crossover Systems
10.35 - 11.00	**Sanchita Goswami, Calcutta University, India** Structural Tuning and Observation of Interesting Magnetic Outcomes in , $\mathrm{Co^{II}Co^{III}}$, $\mathrm{[Mn^{III}].[Mn^{II}Mn^{III}]}$, $\mathrm{Ln^{II}_2}$, $\mathrm{Cu^{II}_4Dy^{III}}$, $\mathrm{Cu^{II}_6Dy^{III}_3}$, $\mathrm{Co^{III}_2Dy^{III}}$, $\mathrm{Co^{III}_2Dy^{III}_2}$, $\mathrm{Co^{II}_2Ln^{III}}$, $\mathrm{Ni^{II}\text{-}Ln^{III}_2}$ and $\mathrm{Cd^{II}\text{-}Ln^{III}}$ Systems
11.15 - 11.45	Tea-Break and Conference Picture - II
Session - 06 (Chair: Srabani Taraphder, IIT Kharagpur)	
11.45 - 12.10	**Muralidharan Shanmugam, University of Manchester, UK** Photo-Chemical Reaction of Cobalt(III)-dioxazolones Characterized by Crystallography, Magnetism and cw/Pulsed EPR Methods.
12.10 - 12.35	**Pratap Vishnoi, JNCASR, India** Linking Structural Dimensionality, Spin-orbit Coupling and Magnetism in Heavy Transition-Metal Halide Double Perovskites
12.35 - 13.00	**Kuduva R Vignesh, IISER Mohali, India** Role of Magnetic Interactions and Diamagnetic 3d Ions on the Magnetic Dynamics of Ln(III) Ions in Homometallic {Dy2} and Heterometallic {3d/4d-4f} SMMs
13.00 - 15.30	Lunch and **Poster Session - II (9th Floor Cafeteria)**
Session - 07 (Chair: Madhab Chandra Das, IIT Kharagpur)	
15.30 - 15.55	**Indra Dasgupta, IACS, India** Spintronics with Rashba Systems
15.55 -16.20	**Ehesan Ali, INST Mohali, India** Molecular Magnetism and Quantum Transport in Sandwiched Complexes
16.20 - 16.45	**Dipak Kumar Goswami, IIT Kharagpur, India** Spin-Crossover Driven Functionalities in OFET Architectures
16.45 - 17.15	Tea-Break

Session - 08 (Chair: Partha Pratim Jana, IIT Kharagpur)	
17.15 - 17.40	**Arpan Mondal, University of Sussex, UK** Reduction of P_4 to $[P_4]^{2-}$, $[P_2]^{2-}$, $[P]^{2-}$ using Masked Divalent Lanthanide Metallocenes
17.40 - 18.05	**Alexey A. Popov, IFW Dresden, Germany** Tuning Magnetic Anisotropy and Metal-Metal Coupling in Endohedral Fullerenes by Exohedral Modification
18.05 - 18.20	Technical Talk: Panalytical
19.30 - 22.30	Conference Dinner (Sky Deck, Taj City Centre, New Town, Kolkata)
Day 3 (December 01, 2025) Monday **Venue: Research Park Lecture Hall (7th Floor)**	
Session - 09 (Chair: Priya Mahadevan, SN Bose National Centre, India)	
09.30 - 09.55	**Mario Ruben, KIT, Germany** Isotopologue Materials: Hilbert Space Engineering of Nuclear-spin Qubits for Implementing Quantum Gates and Quantum Algorithms
09.55 - 10.20	**Abhishake Mondal, IISc Bangalore, India** Switching States: Structural Insights into Light- and Pressure-Induced Bistability
10.20 - 10.45	**Chiranjib Mitra, IISER Kolkata, India** Pulse Schemes for Increasing Coherence Time in an Ensemble of Nitrogen Vacancy Centres in Diamond
10.45 - 11.10	**Suranjan Shil, Manipal Academy of Higher Education, India** Strong Ferromagnetic Coupling between Metal and (Anti)aromatic Radicals via Noncovalent Interaction
11.10 - 11.40	Tea-Break
Session - 10 (Chair: Subhadeep Datta, IACS Kolkata, India)	
11.40 - 12.05	**Rangeet Bhattacharyya, IISER Kolkata, India** Irreversibility of a Stern-Gerlach Experiment
12.05 - 12.30	**Arup Sarkar, Trinity College Dublin, Ireland** Ab Initio Modelling of Spin Coherence in MOF-Hosted Molecular Qubits
12.30 - 12.55	**Amit Kumar Mondal, INST Mohali, India** Spin Selective Electron Transport through Chiral Molecules
12.55 - 13.10	Technical Talk: Agilent Technologies
13.10 - 14.30	Lunch
Session - 11 (Chair: Nitesh Kumar, SN Bose National Centre, India)	
14.30 - 14.55	**Pramod Bhatt, BARC Mumbai, India** Tuning Spin States for Enhanced Magnetic and Electrochemical Functionality in Prussian Blue Analogues
14.55 -15.20	**Sagar Paul, KIT, Germany** Single Molecule Magnets for Quantum Computation: Insights from Micro-SQUID-EPR
15.20 - 15.45	**Alexandre Abhervé, University of Angers, France** Electron's Spin Polarization in Chiral Halide Perovskite Materials
15.45 - 16.10	Valedictory Session
16.10 - 16.40	Tea-Break
19.30 - 22.30	Dinner

Poster Session (Nov 29 and Nov 30)

at the 9th Floor Cafeteria

1	Abhishek Bhardwaj	Vanadyl Quinolinates: Possible Candidates for Qubits
2	Sukanya Guha Roy	Design and Development of Visible Light Active Photocatalysts for Environmental Remediation and Selective Organic Transformation
3	Soumya Satpathi	Phases and phase transtions in 1D alterating mixed spin (½ − 1) chain with frustration and anisotropy
4	Shubhankar Maiti	Optical Insights into Spin-State Switching in Iron(II) Complexes
5	Nilasha Maiti	Low-Temperature Cluster Spin-Glass State in Nickel Hexacyanoferrate
6	Soumyajit Karmakar	Whispers of Coherence: Interfacing Molecular Dynamics and First Principles Calculations to Understand Molecular Qubit Monolayers
7	Sumanta Maity	Anomalous magnetic anisotropy and effects of field cooling in a single 40 nm Fe_3O_4 nanoparticle
8	Abhijit Saha	Photocatalytic Degradation of Azithromycin Using CNC-TiO_2 Nanocomposites: A Sustainable Solution to Antibiotic Pollution and Resistance
9	Dabasish Deka	Cyano-bridged discrete heterometallic dimer and trimers: Synthesis, characterization and magnetic analysis
10	Debopam Sarkar	Engineering Molecular Bistability: Stimuli-Driven Spin-State Switching in Metallosupramolecular Systems
11	Moromi Nath	Spin-Vibrational Relaxation in Cr(V) and V(IV) Tetraphenyl Porphyrin Molecular Spin Qubit Candidates
12	Dhritisundar Paramanik	Probing the Structure-Conductance-Bias Relationship in Atomic Scale Metallic Junctions
13	Kalpita Nath	Effect of salts and electric field perturbations on the internal droplet dynamics of bio-colloidal solutions
14	Dhrubajyoti Mondal	Generalized Heisenberg-Type Magnetic Phenomena in Coordination Polymers with Nickel–Lanthanide Dinuclear Units
15	Prabin Pyakurel Sharma	Modeling of a one-dimensional atomic-scale carbon strip decorated with transition metal adatoms for Magnonic applications
16	Jharna Tamuli	Cyanido bridged $\{Fe_2Ni_2\}$ molecular squares
17	Subhankar De	Electric field driven conformational modifications in metal molecule-metal junction
18	Niku Ahmed	From Magnetic Exchange to Catalytic Efficacy: Unveiling Cyanide Bridged Co-Fe Dimers with Five-Coordinated Co (II) Centre
19	Gaurav Chouhan	Electronic and magnetic phases of a bipartite square-lattice in an extended Hubbard model
20	Anutosh Biswas	Basis Adaptive Algorithm for Quantum Many Body Systems on Quantum Computers
21	Archita Sarkar	Dynamic Molecular Systems: Electron, Spin, and Valence State Modulation
22	Dayal Das	Room-Temperature Near-Infrared Excitons and Optoelectronics in 2D/Organic Heterostructures via Spontaneous Epitaxial Growth

Molecular Spin Qubits toward Quantum Computer Based on Cu(II), Ni(III), Co(II), Fe(III), Mn(II), Cr(V), and V(IV) Complexes with S = 1/2

Masahiro Yamashita[a, b]

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A bit of a conventional computer is composed of a combination of 0 and 1, whereas that of a quantum computer is composed of a superposition of 0 and 1, that is, $\psi = a|0> + b|1>$. Hence, it is called a quantum bit (qubits). Therefore, the quantum computer is drastically superior from the viewpoints of performance, speed, capacity, etc. Qubit candidates for quantum computers are created by using superconducting loops, nitrogen vacancies in diamond, trapped atoms, photons, and quantum dots. These candidates have merits and demerits, such as their coherence time, operating temperature, etc. Therefore, I will focus on molecular spin qubits based on molecular magnets with S = 1/2..

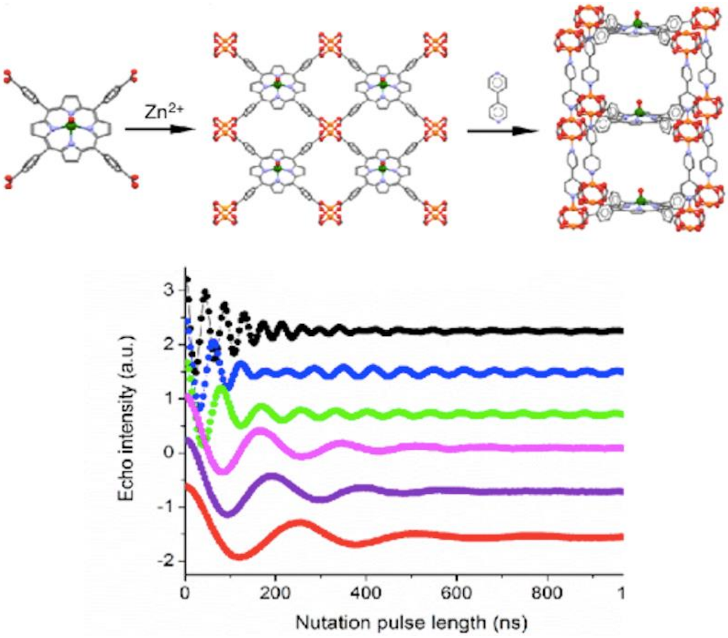

Fig.1. 3D MOF from 0D VO(TCPP) and Rabi Nutation at room temperature.

As for molecular spin qubits for quantum computer, we must increase T_1 (spin-lattice relaxation time) and T_2 (spin-spin relaxation time). Therefore, we will focus on the following three strategies:(1) Crystal Engineering Method; By comparing 0-D [VO(TPP)] and 3-D [VO(TCPP-Zn_2-bpy)], we have investigated the influence of the spin-lattice relaxation (T_1) in 0-D and 3-D lattices. Due to the rigid lattice of 3D-MOF, the Rabi nutation was observed even at room temperature (Fig.1). (2) g-Tensor Engineering Method; By comparing [VO(TPP) and [CrN(TPP)], we have investigated the contribution of the anisotropy of their g-values for the spin relaxation. Due to the large anisotropy of g-values, [CrN(TPP)] shows the shorter life time. (3) Orbital Engineering Method; In order to compare [Ni(cyclam)X_2]ClO_4 and TBA[Ni(mnt)$_2$], we have investigated the relationship between the different occupied orbitals and spin relaxation. [Ni(cyclam)(NO_3)$_2$]ClO_4 has the longer life time due to the rigid molecular structure.

[1] M. Yamashita, S. Roberta, et.al., J. Am. Chem. Soc., 140, 12090-12101(2018)

Single Ion Magnetism in Lanthanide Organophosphates and Phosphonamides

Ramaswamy Murugavel

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Evolving information technology demands energy- and cost-efficient data solutions. Miniaturization has nearly reached its limits, prompting exploration of alternatives like single-molecule magnetism. Over the past 20 years, research in this area has shifted from the use of polynuclear to mononuclear complexes, focusing on how crystal field and molecular symmetry affect the resultant magnetic properties. This has led to highly anisotropic single-ion magnets with improved energy barriers and blocking temperatures. Our group's contributions to this area employing both phosphate esters and phosphonamides as stating materials will be highlighted in this talk.

The authors thank Prof. G. Rajaraman and his group for an active collaboration in modelling our systems. For further details, please refer to our key publications in this area: *Dalton Trans.* **2015**, *44*, 5961; *Chem. Sci.* **2016**, *7*, 5181; *Chem. Commun.* **2016**, *52*, 7168; *Inorg. Chem.* **2017**, *56*, 3946; *Inorg. Chem.* **2017**, *56*, 9071; *Dalton Trans*. **2018**, *47*, 357; *Chem. Commun*. **2018**, *54*, 3685; *Dalton. Trans.* **2019**, *48*, 15928; *Coord. Chem. Rev.* **2022**, *453*, 214288; *Chem. Euro. J.* **2022**, e202103585; *Dalton Trans*. **2023**, *52*, 8943; *Inorg. Chem.* **2023**, *62*, 8435; *Dalton Trans*. **2024**, *53*, 7263. *Inorg. Chem*. **2024**, *63*, 11963; *Chem. Asian J.* **2025**, e202401477

Probing the magnetic properties of actinide complexes by paramagnetic NMR

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The Paramagnetic Nuclear Magnetic Resonance (pNMR) is a powerful tool for probing electronic structure and magnetic properties in paramagnetic systems. While pNMR has been extensively applied to transition metal and lanthanide complexes, its use in actinide chemistry remains relatively under-explored due to the radioactivity of the transuranide complexes. Understanding the pNMR signatures of actinide compounds requires a rigorous theoretical framework that accounts for spin-orbit coupling, magnetic anisotropy, and covalency, while maintaining close synergy with experimental data[1].

Paramagnetic NMR experiments on actinide complexes are performed by Claude Berthon (CEA Marcoule France). In this work, we apply advanced theoretical methods —based on relativistic quantum chemistry, density functional theory (DFT), and wavefunction-based approaches—to model and interpret the pNMR chemical shifts (^{1}H, ^{13}C, ^{15}N, ^{17}O, ^{19}F) of two series of actinide complexes, $[An(NO_3)_6]^{2-}$ and [AnDOTA]L An=U, Np, Pu and L=H_20, F^-.

In complexes with a strong anisotropy, it gives access to the anisotropic magnetic susceptibility $\Delta\chi$.[2,3] In complexes with a compact coordination sphere, it gives access to the spin density at the nuclei of the ligands, and consequently to the ligand hyperfine coupling constants.[3,4] The pathway of the spin density from the magnetic 5f orbitals to the nuclei will be discussed.

For the DOTA series, the primary effect of the apical molecule on the magnetic properties is analyzed. The magnetic susceptibility tensor of the [UDOTA]H_20 complex, calculated from first principles calculation and deduced from pNMR spectroscopy is compared to the torque magnetometry and SQUID experiments performed by the group of Mauro Perfertti (Florence, Italy).

The interplay between experiment and theory is essential in magnetic properties of actinides: theoretical models rely on experimental data for validation, while experimental results require theoretical interpretation to unravel the underlying electronic and magnetic interactions.[5]

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5 “Modeling magnetic properties of actinide complexes” H. Bolvin in Rajaraman, G. (editor) 'Computational Modelling of Molecular Nanomagnets' Springer p 179-218, 2023

Ni(II) Complexes as Electronic Spin Qubits with a Clock Transition

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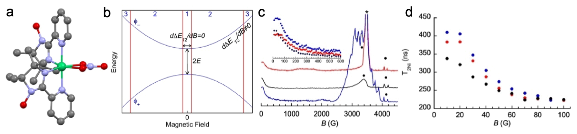
Mononuclear Ni(II) complexes (S = 1) can be engineered to exhibit two closely spaced spin states acting as a two-level system and potential qubit at zero magnetic field, due to their uniaxial magnetic anisotropy (D) and weak rhombicity (E). In the complex illustrated in Figure 1a, the energy gap matches the X-band frequency, enabling a superposition of the two states at zero field—a so-called clock transition.[1]

In this work, we demonstrate that for such mononuclear Ni(II) complexes, the clock transition effectively protects the coherence of the superposed state from spin-bath magnetic fluctuations.[2] To highlight this effect, we compare the coherence time behavior of the Ni(II) complex with that of an iso-structural Co(II) complex (S = 3/2), which lacks such protection due to its half-integer spin (Figure 1). Our results show that increasing the Co(II) concentration within the solid drastically decreases its coherence time, whereas the Ni(II) complex remains largely unaffected.[2]



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Molecular Neuromorphic Building Blocks for Artificial Intelligence

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Artificial Intelligence (AI) has long been a subject of fascination, oscillating between grand promises and inevitable disillusionment. While remarkable milestones, like AI outperforming human champions in complex games, suggest we are entering a new era of computing, a deeper look reveals that these breakthroughs come at a steep cost, demanding vast amounts of energy and intensive, expensive training process. In areas like cognition, decision-making, and intelligence, even our most advanced computing machines fall far short of the brain's unparalleled efficiency and compact design. The core of this challenge lies in the limitations of conventional circuit elements and computing architectures, which struggle to replicate the brain's complex, nonlinear dynamics operating at the edge of chaos. In this seminar, I will introduce a new class of molecular circuit elements designed to capture the intricate, reconfigurable logic that mimics brain-like behaviour at the nanoscale. These devices can be operated as analog or digital elements, or could be poised on the verge of instability, offering a unique potential to emulate neural functions in ways that traditional computing hardware cannot. Our journey explores these molecular systems from their foundational physics and chemistry, all the way to integrated circuit design and on-chip applications [1-8] with the aim of laying the groundwork for AI and machine learning platforms that can transcend the limitations of Moore's Law and lead to a new era of energy-efficient computing.

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Stimuli Responsive Magnetic Molecules

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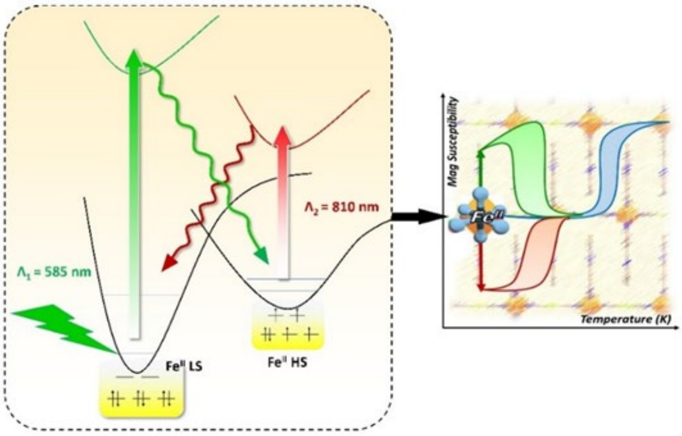
The development of molecular materials that can be switched between two different spin states through the application of external stimuli, e.g., light is of great interest owing to their potential use in molecular devices and information technology[1,2]. This switching behavior can be triggered by different reasons such as a charge/proton transfer, a change in the solid-state structure, or molecular orientation. When the *cooperativity* between spin centres is strong enough, a region of bistability opens, in which either of the two states can be found depending on the material's immediate past. This *memory* effect has been widely exploited in transition metal complexes for their potential application in magnetic data storage, spintronics, sensing etc. Some exciting recent discoveries[3-5] of spin-state switching in the Fe(II) based Hofmann type frameworks and Prussian Blue analogues(PBAs) in presence of external perturbation would be discussed in this presentation.



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Probing the Reliability of Structural Hallmarks in Uranium-Soft Ligand Interactions

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The coordination chemistry of uranium with soft ligands continues to draw interest because of its role in actinide bonding and its relevance to nuclear waste management, separation processes, and materials design. These metal-ligand interactions are often assessed using structural features such as bond lengths, dihedral angles, coordination geometry, and ligand orientation. While these measurements are easy to obtain, they do not always reflect the true picture of chemical bonding or the underlying electronic structure. Part of the challenge comes from uranium's complex electronic configuration. In addition to the 5f orbitals, the 6d, 7s, and even 6p orbitals can participate in bonding, leading to multiconfigurational electronic states and unconventional bonding pattern. As a result, structural metrics alone can be misleading. To get a complete picture, we combine structural descriptions with the observables from multireference quantum chemical methods. This approach helps reveal the details of orbital mixing and covalency, providing a more accurate understanding of uranium-soft ligand coordination.

Modeling Blocking Temperature by Kinetic Monte Carlo Method

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Abstract

Understanding factors that determine the blocking temperature of an assembly of single molecule magnets (SMMs) is essential for controlling this crucial variable as it impacts the technological usefulness of SMMs. This is a daunting problem as it involves dealing with a very large number of degrees of freedom in a nonequilibrium process. As an initial step, we employ the kinetic Monte Carlo method to get insights into the factors that affect blocking temperature. We employ an anisotropic Heisenberg model with diagonal anisotropy for a single SMM and dipolar spin-spin interactions between SMMs. We find that the blocking temperature increases with the strength of dipolar interactions and on the exchange anisotropy of the SMMs. The dipolar interactions become stronger for shorter intermolecular separations, this may be the reason for higher blocking temperatures found in single ion rare earth SMMs.

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In search of 1-dimensional systems, hosting quantum spin liquids

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Magnetic systems are characterised by microscopic interaction strengths that couple magnetic moments of different atomic sites. Depending on the magnitudes, signs, and ranges of these interactions, various magnetic ground states can be realised. Usually, one may estimate the net interaction strength from the temperature-intercept (Θ_{CW}) of the inverse-susceptibility plot as a function of the temperature via the Curie-Weiss Law. This magnitude of Θ_{CW} often provides a good indication of the transition temperature for the magnetic ordering. However, there are many systems where the magnetic ordering temperature is significantly suppressed compared to Θ_{CW} due to frustrations in the magnetic interactions. Alternatively, such frustrated interactions can give rise to a magnetically frozen or glassy state. In some unusual cases, no magnetic ordering or freezing is found down to the lowest temperature probed despite a sizable value of Θ_{CW}, prompting one to believe that such systems host an exotic ground state, known as a quantum spin liquid state.[1] One obvious realisation of such systems would be 1-dimensional magnetic structures, where one is theoretically assured of this phenomenon. However, it has proven to be surprisingly challenging to find suitable approximants of 1-dimensional systems, exhibiting this exotic state, underlining the fact that all physical systems at a sufficiently low energy scale are 3-dimensional. We have been probing several new systems [2] that are probable candidates for this class of compounds, finding experimental features to suggest ground states akin to the quantum spin liquid state with some expected twists in their low-energy properties. I shall present and discuss some of our efforts in this direction.

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Understanding the Quantum Entangled Phases and Quantum Spin Liquid Candidates through Multiscale Modeling

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After a brief introduction to fundamentals of quantum magnetism, I shall discuss a quench dynamics study using density matrix renormalization group (DMRG) method to find many-body localization (MBL) in two-component dipolar fermions subjected to a quasi-periodic potential and finding MBL phases in charge as well as in spin density waves and various other localized and thermal phases [1]. Next, shall discuss our studies on a ferrimagnetic lattice of alternating spin-1 and spin-1/2 chain with nearest neighbour (NN) and next-nearest neighbour (NNN) antiferromagnetic interactions along with the z-component of the Dzyaloshinskii-Moriya (DM) interactions. The linear spin-wave theory and DMRG methods study reveal that these competing exchange and DM interactions introduce strong quantum fluctuations in every lattice site, which in effect destroys the ferrimagnetic order and due to which all the signatures of ferrimagnetism vanish completely [2]. Thereafter, I shall discuss about the possible quantum spin liquid phases in a dimer-based material, $Yb_2Te_5O_{13}$ and in a hyperhoneycomb random lattices, $NaYbW_2O_8$ with two compositions, which were synthesized and thermodynamic and μ-SR studies were carried out by our experimental colleague [3]. In fact, after finding the exchange constants, single ion and biaxial anisotropy parameters, our Monte Carlo based prediction of incommensurate phases at certain temperatures for both the spin lattice systems indicate these as the possible quantum spin liquid (QSL) candidates. In fact, since the neutron scattering data is missing, we have verified our results with the experimental μ-SR data. Many more detail experimental and quantum theoretical studies are necessary to identify these as the elusive quantum spin liquid candidates. Finally, I shall show the nonlinear magneto-electric effect in a toy model (finite size spin-orbital lattice) with tuning the Hubbard interaction term and the spin-orbit coupling interactions [4].

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Role of spin multiplicity of molecular excited states in designing photovoltaics and TADF materials

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Singlet and triplet excited states in organic molecules play an important role in designing photovoltaics and TADF materials. Intermolecular and intramolecular singlet fission mechanism in molecules can reduce the non-radiative energy loss in solar cell and increase cell's efficiency if the energy of lowest singlet excited state (S_1) is nearly close to twice the energy of lowest triplet excited state ($2T_1$)[1,2]. On the other hand, if the lowest excited triplet state (T_1) is nearly close to lowest singlet state (S_1), non-emissive triplet excitons can be repopulated to emissive singlet through Reverse Intersystem Crossing (RISC). This boosts Thermally Activated Delayed Fluorescence (TADF) mechanism in organic Light Emitting Diodes (OLEDs)[3]. This talk will highlight the possible role of such singlet and triplet excited states in some representative organic molecules like diphenyl hexatrienes, B-N substituted pyrene and benzotrithiophene. The excited state calculations are performed based on *abinitio* and model Hamiltonian and are in good agreement with experiments.

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Spin polarised antiferromagnets

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Conventional ferromagnets are characterised by a finite magnetisation, the breaking of time-reversal symmetry, and a spin splitting of the electronic bands, all of which render them highly suitable for spintronic applications. In contrast, antiferromagnets possess zero net magnetisation, and the electronic states with opposite spin orientations remain degenerate, thereby limiting their direct applicability in spintronic devices. Nevertheless, antiferromagnets preserve time-reversal symmetry combined with spatial translation. This talk will focus on a new class of unconventional antiferromagnets which, while retaining vanishing net magnetisation akin to conventional antiferromagnets, simultaneously exhibit spin polarisation of electronic bands in a manner reminiscent of ferromagnets [1-2]. Within a mean-field treatment of the extended Hubbard model on a bipartite lattice, it will be demonstrated that when spin motifs are connected through a rotation under UT symmetry—where *U* and *T* denote SU(2) spin-rotation and translation operators, respectively—the energy bands undergo momentum-space separation, analogous to Rashba-type or anisotropic spin splitting [3]. Conversely, in situations where UT symmetry is broken in the ground state, the Kramer's degeneracy is lifted, giving rise to an isotropic spin splitting, as exemplified in zigzag and honeycomb ladder geometries [4]. These spin-split antiferromagnetic phases represent a promising platform for dissipationless spintronic functionalities.

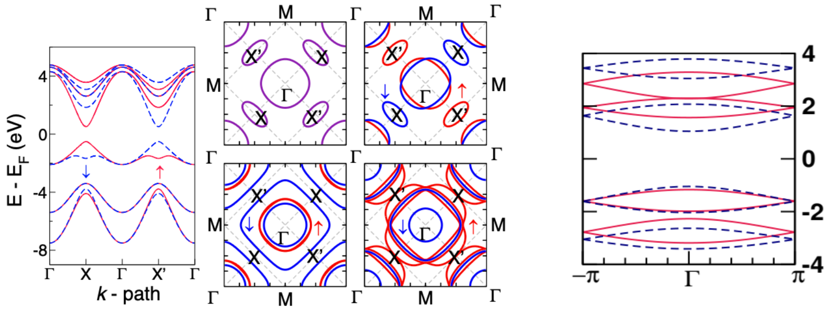

Figure: (Left) Band structure and Fermi surface of bipartite lattice in the charge-ordered antiferromagnetic phase exhibiting anisotropic spin splitting. (Right) Isotropic spin splitting of the band of a honeycomb ladder in the charge-ordered antiferromagnetic phase.

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Speaker: Geetanjali Giri

Title of the talk: Electronic Structure and Spin Dynamics in Multiferroics

Abstract:

This study bridges concepts from **molecular magnetism** and **multiferroics**, as the well-defined exchange pathways and spin–lattice interactions in $GdMn_2O_5$ resemble those observed in molecular magnetic systems. Such parallels provide a molecular-level understanding of the magnetoelectric coupling mechanisms and emphasize how tailored spin interactions can drive complex multiferroic behavior.

Chemical Transformations in Molecular Flasks

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Due to the restricted degree of freedom of chemical entities in confined nanospace their physical and chemical properties are expected to be different from their conventional properties in the bulk medium. Metal ligand dynamic coordination bonds have been extensively used to design discrete metallosupramolecular architectures. My lecture will focus on the design of a few water-soluble Pd(II) discrete molecular architectures that have hydrophobic confined nano-pockets. My lecture will focus on our recent observation on the role of the shape of reaction vessels on the fate of a chemical reaction (Figure 1). By changing the shape of Pd_6 aqueous molecular cages the oxidation of anthrone in presence of water gave different products under the identical reaction conditions. Post-synthesis modification of the cages and encapsulation of photoactive guest for tuning the fate of photocatalytic reactions will be discussed.

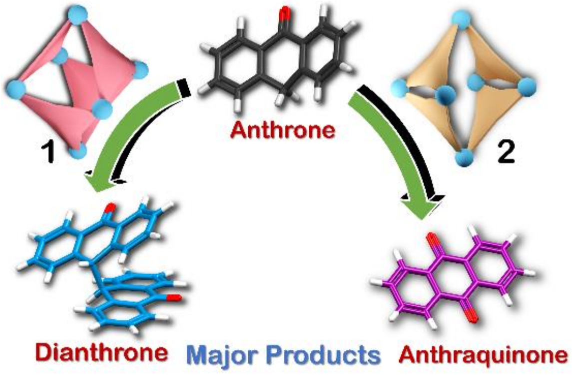

Figure 1. Cavity-shape dependent divergent synthesis.

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Slow Magnetic Relaxation in Spin Crossover Systems

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Molecular magnetism is an attractive field due to its relevance in quantum magnetism, exemplified by single-molecule magnets (SMMs) and molecular spin qubits (MSQs). In this study, we explored the control of slow magnetic relaxation using spin-crossover (SCO) compounds, which allow tunable spin states and molecular distortions. We systematically investigated SMM and MSQ behavior in cobalt(II) ($S = 3/2 \leftrightarrow S = 1/2$) and iron(III) ($S = 5/2 \leftrightarrow S = 1/2$) SCO systems. The representative compounds, $[\mathrm{Co^{II}}_3(\mathrm{dpa})_4\mathrm{Cl}_2]$ (dpa = 2,2′-dipyridylamide anion) and $[\mathrm{Fe^{III}}(\text{diCl-lmn-sal}_2\text{tet})]\mathrm{BPh}_4$ (lmn = 333, 323, 232, 222), were synthesized and characterized by single-crystal X-ray analysis, magnetic susceptibility measurements, and cw/pulsed electron paramagnetic resonance (EPR).

The compounds exhibited diverse spin-state behaviors, ranging from incomplete SCO (HS ↔ HS/LS) and complete SCO (HS ↔ LS) to pure high-spin (HS) and low-spin (LS) states. Distortion parameters (Σ) were compared with those of previously reported SCO Co(II) and Fe(III) complexes, revealing that structural distortions are generally larger in HS states than in LS states. AC magnetic susceptibility measurements at 2 K confirmed frequency-dependent responses, indicative of slow relaxation processes. Furthermore, cw/pulsed EPR studies enabled the estimation of spin–lattice relaxation times (T_1) and coherence time (T_m).

Our results demonstrate that slow magnetic relaxation in the HS state manifests as SMM behavior, while relaxation in the LS state gives rise to MSQ behavior. This work represents the first attempt to establish a molecular design strategy for developing MSQs based on SCO metal complexes, highlighting how tunable spin states and molecular distortions can be leveraged for quantum information applications.

Structural Tuning and Observation of Interesting Magnetic Outcomes in Co^{II}-Co^{III}, $[Mn^{III}].[Mn^{II}Mn^{III}]$, Ln^{III}_2, $Cu^{II}_4Dy^{III}$, $Cu^{II}_6Dy^{III}_3$, , $Co^{III}_2Dy^{III}$, $Co^{III}_2Dy^{III}_2$, $Co^{II}_2Ln^{III}$, Ni^{II}-Ln^{III}_2 and Cd^{II}-Ln^{III} systems

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The quest for molecular magnetic materials possessing potential applications in information storage, spin−dependent electronics and quantum computing is one of the most challenging topics in chemistry, which leads to the generation of single−molecule magnets (SMM) and single ion magnets (SIM). In this context, construction of mixed valence, 4f and 3d-4f entities have witnessed a steady growth as evident by a constantly increasing number of publications in this area.

In this lecture, I wish to provide a glimpse of our laboratory experiences in quest of SMMs/SIMs regarding Co^{II}-Co^{III},[1] $[Mn^{III}].[Mn^{II}Mn^{III}]$,[2] Ln^{III}_2,[3] $Cu^{II}_4Dy^{III}$,[4] $Cu^{II}_6Dy^{III}_3$, $Co^{III}_2Dy^{III}$,[5] $Co^{III}_2Dy^{III}_2$, $Co^{II}_2Ln^{III}$,[6] Ni^{II}-Ln^{III}_2 [7] and Cd^{II}-Ln^{III} systems. A few compounds have exhibited SMM/SIM behavior while a couple of systems depicted slow relaxation of magnetization.

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Photo-Chemical Reaction of Cobalt(III)-dioxazolones Characterized by Crystallography, Magnetism and cw/Pulsed EPR Methods.

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Transition-metal nitrenoid species play a vital role in the synthesis of pharmaceutically important molecules by enabling the formation of C–N, N–N, and other nitrogen-containing heteroatomic bonds.[1] Among the various amino sources commonly used to generate metal–nitrenoid intermediates, such as azides, hydroxylamines, and iminoiodinanes, dioxazolones have emerged as particularly valuable reagents.[2] They not only facilitate the photochemical initiation and control of catalytic processes but also allow access to transient and highly reactive metal–nitrenoid complexes that are otherwise difficult to observe.[3]

A fundamental understanding of the structural and electronic features of these reactive intermediates is essential for elucidating catalytic mechanisms. Such insight provides a foundation for the rational development of next-generation catalysts with improved efficiency, selectivity, and substrate scope. In this study, we present detailed spectroscopic characterization of an open-cubane, high-valent Co(IV)$_3$ cluster (**Figure 1a**) and a mixed-valent Co(III)-Co(IV) species. Furthermore, we describe the generation of a highly unstable Co–nitrene radical intermediate formed via a photochemical reaction between a Co(III)–π-allyl precursor and dioxazolones. The subsequent transformation of this nitrenoid species into a mixed-valent cobalt dimer (**Figure 1b**) is investigated in detail, supported by cw/pulsed-EPR measurements and complementary spectroscopic analyses.[4] Together, these findings provide new insight into the formation, reactivity, and electronic structure of high-valent cobalt nitrenoid intermediates relevant to C–N bond-forming catalysis.

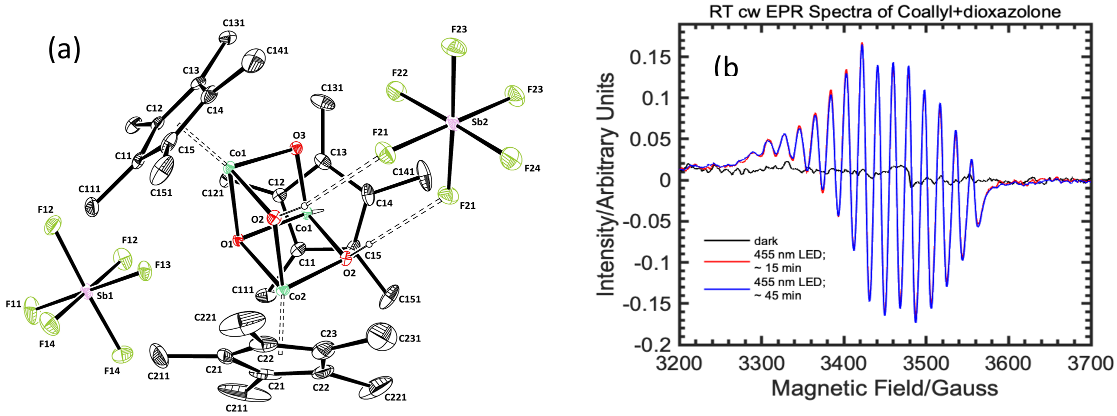

Figure 1. (a) Crystal-structure of open-cubane, high-valent Co(IV)$_3$ cluster and (b) cw-EPR spectra of Co(III)–π-allyl+dioxazolones photoactivated using 455 nm LED

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Linking Structural Dimensionality, Spin-orbit Coupling and Magnetism in Heavy Transition-Metal Halide Double Perovskites

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Over the past decade, magnetic halide perovskites have emerged as a rapidly growing class of materials, attracting significant attention for their rich structural diversity and intriguing magnetic and electronic properties. These compounds bridge the fields of solid-state chemistry and magnetism, offering exciting opportunities for both fundamental understanding and potential applications in areas such as spintronics and quantum materials. This talk will focus on transition-metal halide double perovskites with the general formula $A_2M^{I}M^{III}X_6$ (where A is a large monovalent cation, M^{I} is a univalent metal cation, M^{III} is a trivalent metal cation, and X is a halide anion), along with their related structures. I will outline our approach to designing such perovskites with tailored composition and structural dimensionality. I will then share our work on Mo-based halide double perovskites, one-dimensional chain $(CH_3NH_3)_2M^{I}M^{III}X_6$ (M^{I} = Na or Ag; M^{III} = Mo, X = Cl, Br or Cl-Br alloyed) and two-dimensional halide perovskites, $A^{1+}{}_4M^{I}Mo^{III}X_8$ and $A^{2+}{}_2M^{I}Mo^{III}X_8$, ($M^{I}$ = Na, Ag; A^{1+}/A^{2+} = organic ammonium cation; X = Cl, Br). These materials show dimensionality- and composition-dependent antiferromagnetic magnetic exchange interactions. This talk will also cover vacancy-ordered $A_2Ru^{IV}X_6$ (A = K, NH_4, Rb, Cs, CH_3NH_3; X = Cl, Br), which enabled us to estimate the strength of spin-orbit coupling (SOC) based on their single-ion magnetic study.

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Role of magnetic interactions and diamagnetic 3d ions on the magnetic dynamics of Ln(III) ions in homometallic {Dy_2} and heterometallic {3d/4d-4f} single-molecule magnets

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Single-molecule magnets (SMMs) are discrete molecules capable of retaining their magnetization even in the absence of a magnetic field, which gives rise to magnetic hysteresis at a molecular level and an ability to act as magnets below their blocking temperature (T_B).[1] These SMMs have several exciting potential applications, such as information storage devices, Qubits, and spintronics devices. The requirement of high magnetic anisotropy and strong magnetic coupling to enhance the performance of SMMs has led our interest to focus on lanthanide (Ln)-based and heterometallic {3d-4f} and {4d-4f} complexes.[2] The synthesis and modeling of spin-Hamiltonian parameters (such as magnetic exchange coupling (J), and g–tensors) in mono- and dinuclear lanthanide (Ln) complexes, mixed {3d-4f} and {4d-4f} complexes using both experimental and computational tools to understand their molecular magnetic behavior will be discussed. Single-ion Dy(III) examples were made in our lab, showing large thermal anisotropy barriers to magnetic reversal. The role of diamagnetic 3d ions and the bridging ions such as oxide, peroxide, and hydroxide in heterometallic 3d-4f complexes has also been investigated.[3] The effect of J has on the SMM properties of dinuclear Ln complexes and several heterometallic 3d-4f/4d-4f complexes have been probed.[3,4]

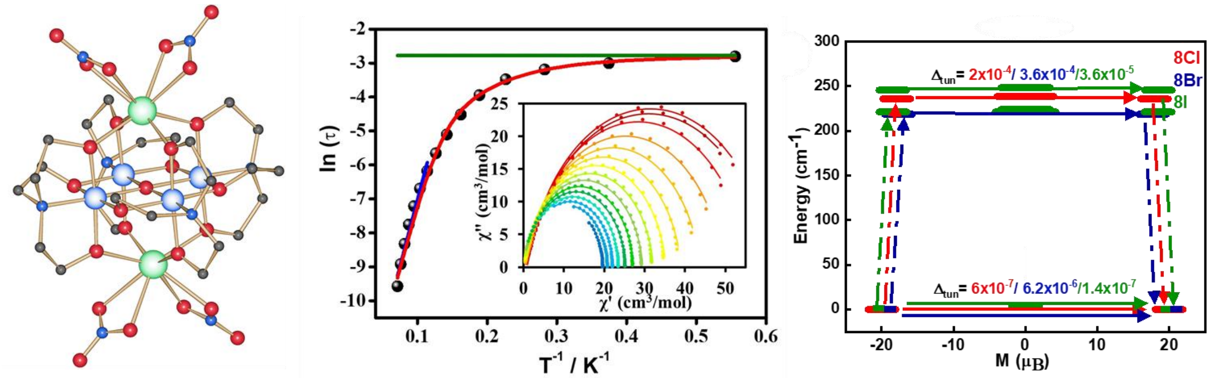

Figure. (left) Molecular structure of {$Co^{III}_4Dy^{III}_2$} SMM; (middle) Magnetization relaxation time (τ), plotted as ln(τ) vs. T^{-1} for a {Dy^{III}_2} SMM. (Inset) Cole−Cole plots between 1.8 and 14 K. (right) *Ab initio* computed magnetic relaxation of {$Dy^{III}_2X_2$} (X = halides) complexes.

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Spintronics with Rashba Systems

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In non-centrosymmetric systems, the non-vanishing gradient of the electrostatic potential results in a momentum dependent magnetic field in the rest frame of the electrons. The coupling of this field with the spin of the electron lifts the spin-degeneracy of the bands in an otherwise non-magnetic system and also leads to complex spin textures in the reciprocal space. Spin textures depending on the symmetry may display Rashba, Dresselhaus, persistent or more complex spin configurations that are important for application in spintronics. We shall show from symmetry considerations that in nonpolar chiral systems, bands with specific orbital characters around a high-symmetry point with D_2 little group may admit a single spin-dependent term in the low-energy model Hamiltonian that naturally leads to persistent spin texture (PST). Considering a two-dimensional plane in the Brillouin zone, we have further argued that in such chiral systems, the PST is transpired due to the comparable strengths of the Dresselhaus and Weyl (radial) interaction parameters where the presence of these two terms is allowed by the D_2 symmetry. Next, we show in a polar compound Ta_2CS_2, a representative member of the MXene family, local symmetries and orbital compositions are responsible for the nontrivial band splitting displaying characteristic spin textures at various high-symmetry points in the Brillouin zone. First-principles calculations, supplemented by a $\mathbf{k}\cdot\mathbf{p}$ model Hamiltonian, demonstrate the presence of both linear and higher-order Rashba terms at the Brillouin zone (BZ) center Γ, where the system exhibits little-group symmetry C_{3v}. Additionally, we observe valley-dependent Zeeman-type spin splitting at the non-time-reversal invariant momentum (TRIM) points K and K'. Furthermore, we identify that the opposite spin splitting at the K and K' points arise from a complex orbital composition that induces an intrinsic orbital moment, influencing the nature of spin splitting and is important for spin-orbitronics. Finally we show such systems with novel spin textures can display intrinsic spin Hall effect.

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Molecular Magnetism and Quantum Transport in Sandwiched Complexes

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This work presents a dual focus on molecular magnetism and molecular spintronics. We first address a critical challenge in single-molecule magnets (SMMs): the lower magnetic anisotropy typically observed in Erbium(III) (Er3+) SMMs compared to Dy3+ analogues, stemming from Er3+'s prolate electronic density. We have computationally investigated heteroleptic Er(III) sandwich complexes, successfully tuning the ligand field by replacing a carbon atom with various heteroatoms in the five-membered ring. Our *ab initio* calculations demonstrate that the resulting structural distortion and modified electronic structure effectively adjust the magnetic axis and significantly improve the magnetic relaxation barrier, providing a vital strategy for designing high-performance Er-based SMMs.[1-3] Building on these fundamental material science insights, the discussion transitions to device-level application by presenting quantum transport calculations for a prototype device: a sandwiched $TbPc_2$ SMM attached to gold leads. Specifically, we will detail how the robust magnetic state of TbPc2 can be used to control quantum interference effects, which is a critical mechanism for engineering electrically addressable molecular spintronic devices such as high-efficiency spin filters and memory elements.[4]

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Spin-Crossover Driven Functionalities in OFET Architectures

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Molecular spin-state dynamics offer a powerful route to engineer responsive organic electronic devices. This work harnesses spin-crossover (SCO) transitions, reversible switching between low-spin and high-spin states, in 1D triazole-based Fe(II) polymers and 3D Hofmann-type Fe(II)(pyrazine)[Pd(CN)$_4$] frameworks embedded as dielectric layers in OFET architectures. These coordination systems exhibit strong cooperativity and sharp dielectric transitions, producing extraordinary capacitance jumps (~1100 nF/cm^2) and loss-tangent switching near their transition temperatures. Integrating SCO materials into OFETs yields temperature-dependent mobility modulation, threshold-voltage shifts, dual-slope transfer behavior, and pronounced hysteresis—signatures of trap redistribution, dielectric reorganization, and order–disorder processes accompanying spin-state conversion. SCO-MOFs further enhance tunability through capacitive hysteresis, frequency-selective dielectric response, and ferroelectric-like domain activity. Together, these results establish molecular spin crossover as a functional degree of freedom for tailoring charge transport, dielectric properties, and memory effects in organic electronics, enabling pathways toward reconfigurable logic, neuromorphic elements, and spin-adaptive sensors.

Reduction of P_4 to $[P_4]^{2-}$, $[P_2]^{2-}$, $[P]^{2-}$ using Masked Divalent Lanthanide Metallocenes

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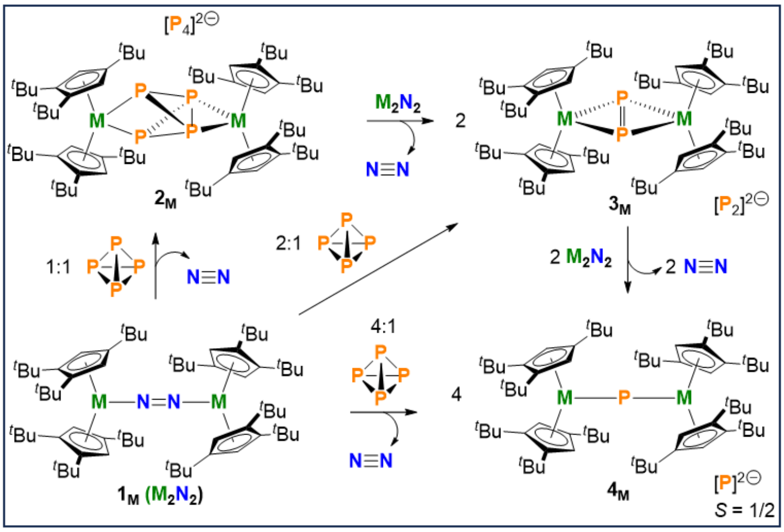
Recently, divalent lanthanide metallocenes have attracted significant attention due to their single-molecule magnet (SMM) behaviour and small molecule activation chemistry.[1] In this regard, the isolation of dinitrogen bridged complexes obtained from N_2 activation and the study of their magnetic properties are well known for f-element chemistry. In contrast, the diphosphorus bridged lanthanide complexes are extremely rare.[2] In this work, we have isolated rare diphosphorus and phosphorus radical bridged lanthanide metallocenes from P_4 activation using masked divalent dinitrogen bridged lanthanide complex. The reaction between P_4 and $[\{(\mathrm{Cp^{ttt}})_2\mathrm{Ln}\}_2(\mu\text{-}\eta^1{:}\eta^1\text{-}\mathrm{N}_2)]$ ($\mathbf{1_M}$), (where M= Y, Gd, Dy, $\mathrm{Cp^{ttt}}$ = 1,2,4-tri-tert-butylcyclopentadienyl) with proper stoichiometry results in the formation of $[\{(\mathrm{Cp^{ttt}})_2\mathrm{Ln}\}_2(\mu\text{-}\eta^2{:}\eta^2\text{-}\mathrm{P}_4)]$ ($\mathbf{2_M}$), $[\{(\mathrm{Cp^{ttt}})_2\mathrm{Ln}\}_2(\mu\text{-}\eta^2{:}\eta^2\text{-}\mathrm{P}_2)]$ ($\mathbf{3_M}$), and $[\{(\mathrm{Cp^{ttt}})_2\mathrm{Ln}\}_2(\mu\text{-P})]$ ($\mathbf{4_M}$) complexes (Scheme 1). Structural analysis reveals that Ln-P bond distance is in the range of 3.054(3)-2.7686(3) Å and decreases from complex $\mathbf{2_M}$ to $\mathbf{4_M}$. In complex $\mathbf{3_M}$, the P-P distance is in the range of 2.0387(6)-2.049(3) Å. Notably, the complexes $\mathbf{3_M}$ and $\mathbf{4_M}$ represent the first example of side-on diphosphorus and divalent P-radical based lanthanide complexes respectively. The magnetic studies reveal the presence of weak ferromagnetic exchange interaction between two $\mathrm{Gd^{III}}$ centres in $\mathbf{2_M}$ ($J_{\text{Gd-Gd}}$ = +0.40 $\mathrm{cm^{-1}}$) whereas antiferromagnetic exchange interactions were observed for complexes $\mathbf{3_M}$ ($J_{\text{Gd-Gd}}$ = -1.02 $\mathrm{cm^{-1}}$) and $\mathbf{4_M}$ ($J_{\text{Gd-Rad}}$ = -28 $\mathrm{cm^{-1}}$, $J_{\text{Gd-Gd}}$ = -1.67 $\mathrm{cm^{-1}}$).



Scheme 1. Synthesis of $[P_4]^{2-}$, $[P_2]^{2-}$, $[P]^{2-}$ bridged lanthanide complexes.

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Tuning magnetic anisotropy and metal-metal coupling in endohedral fullerenes by exohedral modification

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Metallofullerenes with endohedral lanthanides emerged as a versatile class of single-molecule magnets owing to the strong single-ion magnetic anisotropy and peculiar metal-metal interactions, which can be realized in the interior of the fullerene cage. Since exohedral chemical modification of fullerenes is often used to adjust their properties and processability for prospective practical applications, it is necessary to understand how it can affect magnetic properties of EMFs.

In this work we studied how a popular [2+1] cycloaddition reaction, photochemical addition of adamantylidene (Ad), affects single-ion magnetic anisotropy and single-molecule magnetism of $MSc_2N@C_{80}$ (M = Nd, Dy), $Dy_2ScN@C_{80}$, and $Dy_3N@C_{80}$. For each fullerene, reaction yielded [5,6]-open and [6,6]-open isomers of monoadduct $M_3N@C_{80}$(Ad). Paramagnetic ^{1}H NMR was found to be a convenient and powerful tool for determination of the orientation of endohedral cluster with respect to the Ad moiety. *Ab initio* calculations and Nd-based photoluminescence showed that the [5,6] isomer has enhanced ligand-field splitting, whereas coordination of lanthanide to the Ad-addition site in the [6,6] isomer reduces magnetic axiality and ligand field splitting.

SQUID magnetometry and relaxation measurements demonstrated that for $DySc_2N@C_{80}$(Ad), Dy-Ad coordination leads to the noticeable reduction of the blocking temperature of magnetization, whereas Dy coordination to the unfunctionalized fragments of the fullerene cage improves SMM performance in comparison to the unfunctionalized $DySc_2N@C_{80}$. For $Dy_2ScN@C_{80}$, Ad addition has almost no effect on the strength of the Dy···Dy coupling in the [6,6] isomer of $Dy_2ScN@C_{80}$(Ad), but does increase the coupling in the [5,6] counterpart by 20%. For $Dy_3N@C_{80}$(Ad), Ad addition substantially increased Dy···Dy coupling constants and the energy spread of exchange-coupled states in comparison to $Dy_3N@C_{80}$ and lifted geometric frustration. As a result, both $Dy_3N@C_{80}$(Ad) isomers exhibit open hysteresis without pronounced QTM signatures and have higher blocking temperature of magnetization than the pristine $Dy_3N@C_{80}$. Our work demonstrates that chemical derivatization can have profound influence on the single-ion magnetic anisotropy and metal-metal coupling metallofullerene molecular magnets. Thus, chemical derivatization of EMFs can become a useful tool for improving their magnetic properties, but will require careful evaluation of different factors for each reaction type.

Isotopologue Materials: Hilbert Space Engineering of Nuclear-spin Qubits for Implementing Quantum Gates and Quantum Algorithms

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The nuclear spin degree of freedom in rare-earth molecules will be proposed to act as quantum registers for Quantum Computing (QC) and Quantum Communication (QComm). We report on the implementation of lanthanide metal complexes into nanometre-sized spintronic devices by a combination of bottom-up self-assembly and top-down lithography techniques. The controlled generation of magnetic molecular nanostructures will be shown and persistence of their magnetic properties under confinement will be confirmed. The Hilbert space spanned by the nuclear spins will be engineered synthetically and addressed both electrically 1-11 and optically,12-13 partially at the single molecule level.1-13 Finally, Grover´s quantum search algorithm will be implemented on the nuclear spin register of a TbPc2 Qudit.10

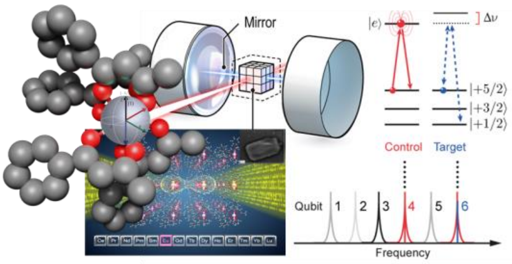

Figure 1. *Representation of the structure and optically addressing rare-earth molecular qubits, here Europium(III), taken from [13].*

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Switching States: Structural Insights into Light- and Pressure-Induced Bistability

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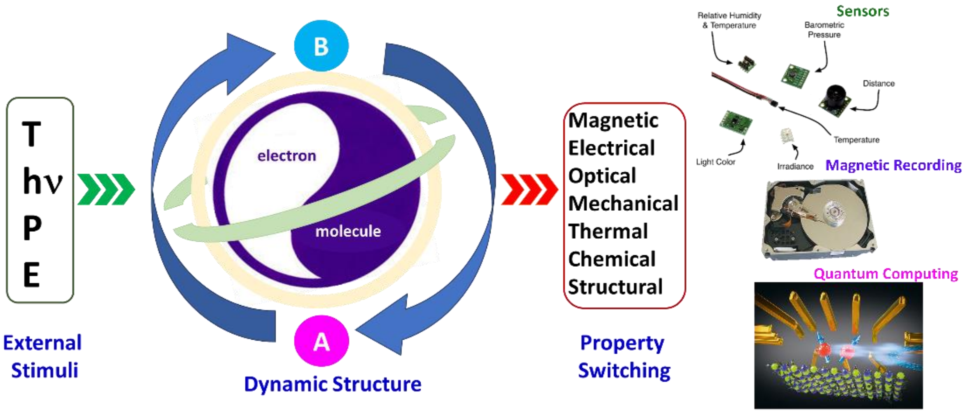
Stimuli-responsive molecular magnetic materials can reversibly switch between electronic and magnetic states under light irradiation, temperature, or pressure changes.[1, 2] These transformations emerge from a subtle balance between molecular electronic structure and collective lattice dynamics.[3] To unravel this interplay, crystallography captures structural distortions while spectroscopy traces spin and orbital rearrangements.[4, 5] Molecular bistable systems—capable of existing in two distinct spin or structural states—represent a particularly promising class of materials, bridging the gap between molecular design and functional magnetic behavior.



In this talk, I will focus on the development and study of stimuli-responsive molecular bistable systems that exhibit controllable spin-state switching under external perturbations such as light and pressure.[6, 7, 8, 9] Light-induced excitation and pressure modulation provide orthogonal and tunable means to manipulate the molecular and electronic structure, offering direct insight into the coupling between structure, spin state, and magnetic properties. I will highlight recent investigations on mononuclear Fe(II) complexes and cyanide-bridged Mo–Fe assemblies, demonstrating how external stimuli govern their spin transitions and structural reorganizations. These studies reveal the subtle interplay between crystal packing, ligand field strength, and cooperative interactions, thereby elucidating fundamental design principles for achieving reversible, switchable, and robust molecular magnetic materials.

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Pulse schemes for increasing coherence time in an ensemble of nitrogen vacancy centres in diamond

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Abstract:

One of the main challenges in quantum information processing (QIP) is to fabricate qubits which can function as quantum memories for considerable amount of time, so that one can perform the gate operations faster than it takes the qubits to decohere. Nitrogen vacancy (NV) centers can provide reasonably long coherence times and their spin photon interface can enable one to entangle two sets of spin ensembles over long distances, thereby not only offering larger Hilbert spaces for computation, but also a mechanism for connecting different quantum computing nodes, increasing the scalability with ease. These systems also offer an amalgamation of electron spin qubit and nuclear spin qubits, through hyperfine interactions which can be controlled through a combination of optical and microwave pulses. However, the spin environment in an ensemble of NV centres can cause the spin-spin relaxation time (T2) to be reduced significantly that can affect the coherence time. We have made suitable dynamical decoupling schemes to isolate the effect of the bath which increases T2 significantly. Once such scheme is known as the Carr-Purcell-Meiboom-Gill (CPMG) pulse scheme, where a string of pulses are applied at equal time intervals. We have implemented this pulse sequence in our NV center ensemble system and observed decoherence suppression across multiple orders of magnitude. We have also managed to explain the reduction in decoherence considering Spin-Boson Model, where one can demonstrated that applying consecutive short ? pulses can suppress the decoherence of a qubit, typically leading to an exponential decay of the signal [1].

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Strong Ferromagnetic Coupling between Metal and (Anti)aromatic Radicals via Noncovalent Interaction

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We have aimed to understand the interaction between the odd electron aromatic or antiaromatic radicals with cobalt and its dipositive ion to understand the magnetic interaction between them. The Density Functional Theory (DFT) along with Complete Active Space Self Consistent Field (CASSCF) method has been used to calculate the magnetic interaction between the radical molecules and the metal (Co/Co^{+2}). The results of this work signifies that the odd electron (anti)aromatic based magnetic molecules could be useful as strong low-dimensional magnetic materials. The Non-Covalent Interaction (NCI) and Electron Localization Function (ELF) analysis indicates that there is no covalent bonding between radicals and the metal. The absence of covalent bonding between the metal and radicals indicates direct ferromagnetic interaction between them. Aromaticity in the studied Co/Co^{+2}–radical complexes has been evaluated using Nucleus Independent Chemical Shift (NICS), Harmonic Oscillator Model of Aromaticity (HOMA), and Gauge-Including Magnetically Induced Currents (GIMIC) analysis, revealing a complex, multidimensional nature of aromaticity. NICS(1) values indicated that the same ring exhibit both aromatic and antiaromatic behavior, depending on the spatial orientation of the metal center. These observations highlight the need for multiple aromaticity descriptors to fully capture the complex aromatic character of these systems.

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Irreversibility of a Stern-Gerlach experiment

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The Stern-Gerlach experiment (SGE) has been known for decades, but a complete theory that explains all facets of it remains enigmatic. In its classic realization, each spin state of an atom follows a unique path or trajectory in an SGE. The enigmatic part is the final output of SGE. Feynman envisaged the outcome to be an entangled state, a superposition of |spin state>⊗|corresponding path>. Later works described the final state of SGE as a mixed state, a weighted average of states belonging to separate beams or trajectories. Notably, Schwinger, Englert, and Scully compared the difficulty of obtaining a coherent output (a pure state) to "putting together Humpty Dumpty" again. Yet recent experiments using Bose-Einstein condensates indicate the emerging beams are partly coherent, favoring Feynman's description. In this work, we revisit SGE using a recent version of the quantum master equation. We show that both outcomes are probable depending on the time of flight and the timescale of the environmental fluctuations. We predict that the output is initially coherent and grows gradually into a mixed state. Moreover, we also estimate how the magnetic-field gradient helps broaden the beam waist. Moreover, our treatment implies that the wave function of an atom passing through a Stern-Gerlach device does not undergo an instantaneous collapse; rather, a gradual decay of coherences results in a mixed state, resulting in an irreversible process.

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Ab Initio Modelling of Spin Coherence in MOF-Hosted Molecular Qubits

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Molecular qubits hosted by metal-organic frameworks (MOFs) represent one of the latest frontiers of spin-based quantum sensors or qubits, where long spin coherence times are combined with chemical versatility. The electronic states and vibrational modes of these frameworks carry sufficient information, which eventually exhibit long coherence time to behave as qubits. Here we employed ab initio spin relaxation theory to fully investigate the role of one- and two-phonon processes to understand the spin-phonon relaxation of vanadyl tetraphenylporphyrinate MOF, namely in [VO(TCPP-Zn_2-bpy)].[1] Here, we employed the fourth-order contributions to the two-phonon processes[2] to simulate the spin-lattice relaxation time (T_1) using NEVPT2(1,5) and NEVPT2(9,9) methods. Expanding the active space from d-d excitations to metal-ligand bonding orbitals[3] clearly shows an improvement in the spin-dynamics, emphasizing the use of the full electronic Hamiltonian instead of the effective Hamiltonian formalism, where the latter is often used as a standard method in lanthanide complexes.

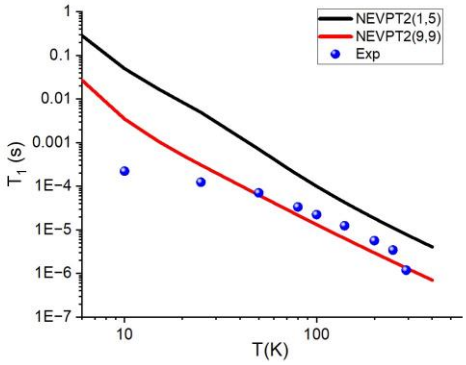

Figure: Comparison of the experimental and ab initio spin-lattice relaxation time (T_1) for the VOTCPP MOF using different active spaces.

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Spin Selective Electron Transport through Chiral Molecules

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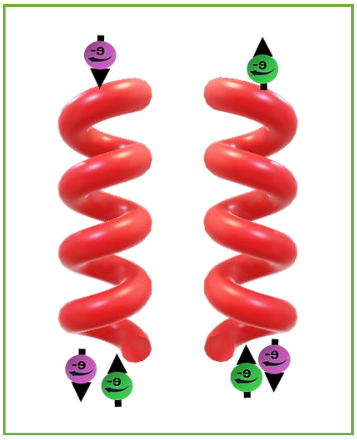
Recent experiments have demonstrated that the electron transfer through chiral molecules depends on the electron spin orientation. This phenomenon has been termed the chiral-induced spin selectivity (CISS) effect,[1] and it provides a challenge to theory and promise for organic/inorganic molecule-based spintronic devices. Recently an efficient method to organic spintronic based on CISS effect has been suggested.[2] In the CISS effect, the chirality of the molecular system itself acts as a spin-filter, thus avoiding the use of magnets for spin injection. Techniques for measuring spin-selective electron transport through molecules and some examples of recent experiments will be discussed.[3-6] By studying spin-dependent electron transport through various bio-molecules (like DNA, peptides, proteins, etc), supramolecular structures, organic/inorganic chiral molecules, we can able to describe the possible application of the CISS effect for developing new kinds of memory devices. Such memory would be based on spintronics, the use of the electrons' spin, rather than charge. Furthermore, the CISS effect is a multidisciplinary phenomenon with implications in chemistry, physics and biology; therefore, this field has many-fold directions and will open new avenues for scientific and technological exploration.



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Tuning Spin States for Enhanced Magnetic and Electrochemical Functionality in Prussian Blue Analogues

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Recent progress in molecule-based magnetism has revitalized interest in designing and understanding functional molecular materials with tunable spin and electronic properties. Among these, Prussian Blue Analogues (PBAs) have emerged as exemplary molecular magnets owing to their flexible cubic frameworks, rich electronic configurations, and compositional tunability [1-4]. These materials exhibit a remarkable combination of properties, including magneto-optical switching, photoinduced charge transfer, ion sensing, electrocatalysis, and reversible ion storage.

This presentation focuses on establishing a direct correlation between the crystal structure, spin states, and multifunctional behavior of PBAs. Emphasis is placed on strategic tuning of spin configurations and magnetic interactions through external stimuli—such as temperature, pressure, and magnetic field—as well as through controlled engineering of structural vacancies and transition-metal compositions. The discussion further highlights how optimized porosity and vacancy concentration can synergistically enhance both magnetic performance and electrochemical functionality, making PBAs promising candidates for next-generation molecular magnets and advanced energy storage systems.

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Single Molecule Magnets for Quantum Computation: Insights from Micro-SQUID-EPR

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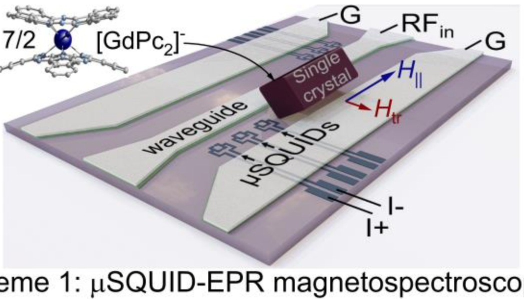
Single-molecule magnets (SMMs) possess robust quantum states that can be reproducibly prepared and tuned by engineering magnetic anisotropy at the molecular level. These systems can exhibit ultraslow relaxation [1] and resonant quantum tunneling of magnetization (QTM), enabling a wide range of quantum applications [2]—from quantum sensing and memory to multilevel quantum bits (qudits) and fault-tolerant quantum computation. The hyperfine levels detected via micro-SQUID ($M(H)$) measurements and single-electron-spin-transistors, which enable nuclear spin-based quantum computation [3], along with observations of long decoherence times for electronic spin states in single-ion magnets [4], have reignited interest in these systems. A detailed mapping of the spin manifold in SMMs—via orientation and frequency scans—is vital for their integration into quantum technologies. The combined micro-SQUID-EPR technique [5] uniquely probes spin states by exciting single crystals with microwaves while simultaneously measuring magnetism (Scheme. 1). Using this method, $M(H)$ loops recorded across the 30 mK–5 K range and under varying microwave frequencies reveal absorption peaks corresponding to specific spin transitions. Plotting these peak positions against RF frequency (0.1–40 GHz) and field orientation enables full reconstruction of the system's spin Hamiltonian [5] and direct observation of anti-level crossings between spin states. The latter has recently enabled a spectroscopic pathway to directly visualize topologically quenched tunneling regimes—a manifestations of geometric phase in spin-systems, advancing prospects for holonomic, fault-tolerant quantum computation based on 4f-SMMs.



Scheme 1: μSQUID-EPR magnetospectroscopy

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Electron's Spin Polarization in Chiral Halide Perovskite Materials

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By combining the optoelectronic properties of halide perovskites (HPs) with chirality from inserted organic cations, chiral HPs brought new perspectives for chiroptical properties, such as circularly polarized luminescence (CPL), or spintronic devices such as spin valves or spin-LEDs, since chiral molecules can substitute ferromagnetic materials thanks to the chirality-induced spin selectivity (CISS) effect. We first revealed both experimentally (mc-AFM) and theoretically (band structure and spin texture calculations) the influence of crystal symmetry elements on the spin polarization ability of this family of materials [1]. It ultimately allowed us to describe a spin-valve device based on the CISS effect. More recently, we reported a full series of lead-free chiral double perovskites [2]. In combination with their lead-based counterparts, such series will ultimately allow us to investigate the fundamental role of metal ions on the CISS effect. On the other hand, revealing the chiroptical behavior of chiral HPs require a proper characterization of circular dichroism (CD) and CPL in the solid state, considering the macroscopic interferences inherent to highly crystalline thin films. An experimental guide to accurately discriminate between both intrinsic CD/CPL and macroscopic effects was recently reported with the example of 1D chiral lead-halides [3].

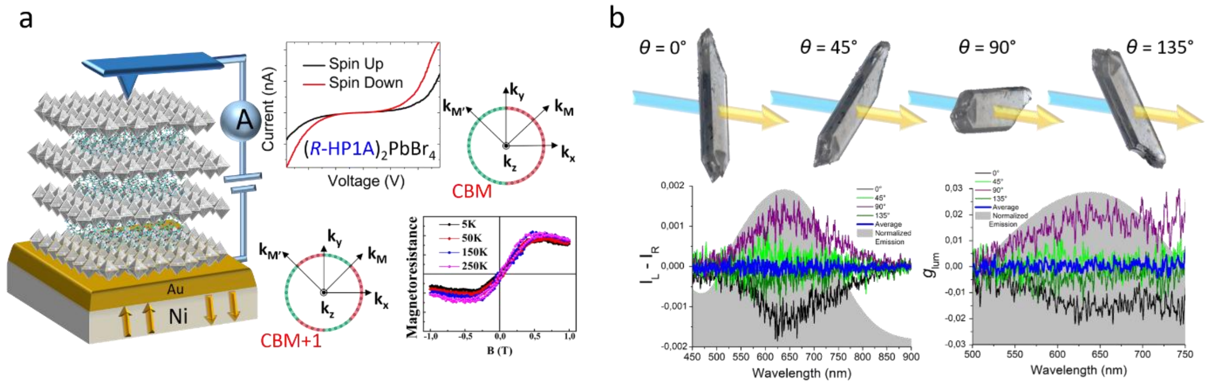

Figure | a) Spin polarization in a 2D lead-bromide perovskite. b) CPL in 1D lead-bromide network.

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Vanadyl Quinolinates: Possible Candidates for Qubits

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Molecular spin systems, particularly vanadium(IV) complexes, offer tunable qubits with long coherence times due to d-orbital splitting and a single unpaired electron.[1-3] Unlike silicon and diamond defect systems, their interactions can be precisely controlled through synthetic design, making them promising candidates for quantum technologies.[4-6] Herein, we report the synthesis and detailed characterization of a new oxovanadium(IV) complex, vanadium oxo bis(8-hydroxyquinoline-2-carbaldehyde) $[VO(Q\text{-}CHO)_2]$ (**1**), as a potential qubit material. Comprehensive analysis using single-crystal X-ray diffraction and electron spin resonance (ESR) spectroscopy, including pulse-EPR studies, revealed significant spin relaxation (T_1) and phase memory times (T_m) ranging from 0.184 to 0.606 μs at 5.0 K across various resonant pulse fields, surpassing similar systems (Figure 1). The unique coordination geometry around V(IV) is attributed to these enhanced coherence properties. Efforts are underway to further modify the aldehyde moiety into Schiff bases with various amines to enhance coherence times, offering insights into molecular design strategies for optimized qubit performance.

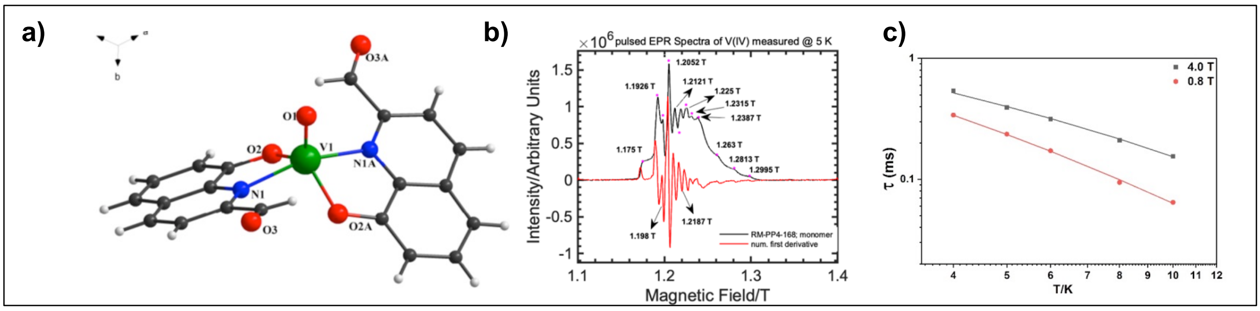

Figure 1. a) Molecular structure of $[VO(Q\text{-}CHO)_2]$ (**1**), b) EDFS spectra of a polycrystalline sample of **1** recorded at 5.0 K, and c) Temperature dependence of τ extracted from ac susceptibility measurements for compound **1** at different applied static magnetic field values.

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The pulse EPR studies were done in collaboration with Dr. Muralidharan Shanmugam & Prof. Eric J.L. McInnes.

Synthesis and characterization of $NiFe_2O_4@Ag_2CO_3$ hybrid for photodegradation of ciprofloxacin and norfloxacin

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The popularity of heterostructured photocatalysts has been steadily increasing since their emergence, owing to their enhanced interfacial charge transfer, tunable band structures, and superior visible-light activity. In this work, $NiFe_2O_4@Ag_2CO_3$ ($NFO@Ag_2CO_3$) photocatalyst was prepared by a simple self-assembly method for the efficient degradation of ciprofloxacin (CIP) and norfloxacin (NOR). The catalysts were characterised by PXRD, UV-vis DRS spectrum, SEM, XPS, BET, FTIR, EPR. The NFO nanoparticles were attached on the surface of Ag_2CO_3 nanorods synthesized by low temperature precipitation method, resulting a unique 0D/1D morphology, which increased the number of active sites. Due to introduction of magnetic NFO, $NFO@Ag_2CO_3$ exhibited excellent magnetic recovery performance. The mass fraction of NFO was 5% and the degradation efficiency of composite photocatalyst was the highest (84 % for CIP and 63 % for NOR) as compared to pure NFO and Ag_2CO_3. Control studies suggested the predominant involvement of superoxide radicals ($O_2^{\bullet -}$) followed by holes (h^+) and hydroxyl radicals ($OH^{\bullet}$) respectively. The improved photoactivity of $NFO@Ag_2CO_3$ should be attributed to the construction of heterojunction with tight interface, which boosts the separation and transfer of photoinduced electron and hole pairs.

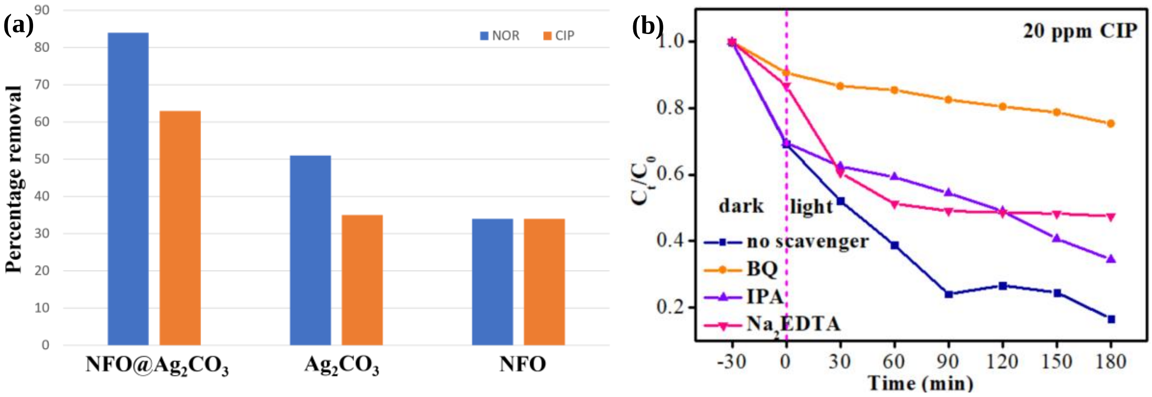

Figure 1 – (a) Histogram of % removal of CIP and NOR by $NFO@Ag_2CO_3$ composite, Ag_2CO_3 and NFO (b) Photocatalytic degradation kinetics of CIP by $NFO@Ag_2CO_3$ composite in presence of radical scavengers.

Phases and phase transtions in 1D alterating mixed spin (½ − 1) chain with frustration and anisotropy

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We investigate the one-dimensional alternating mixed-spin (1/2 – 1) chain in the presence of both frustration and anisotropy. Frustration is introduced via next-nearest-neighbour interactions, while anisotropy is incorporated at each lattice site. Our results show that moderate frustration can drive a phase transition from a ferrimagnetic to an antiferromagnetic ground state. Remarkably, even a weak easy-plane anisotropy is sufficient to destabilize the ferrimagnetic order. Under strong frustration and anisotropy, the system exhibits signatures of a possible spin-density wave (SDW) phase. To explore these phenomena, we employ exact diagonalization (ED) for small system sizes and the density matrix renormalization group (DMRG) method to characterize ground state properties in larger systems. Finite-temperature behaviour across various phases is studied using the ancilla-based time-evolving block decimation (TEBD) approach. Our primary objective is to elucidate the phase structure of alternating mixed-spin chains under the combined effects of frustration and anisotropy. These findings contribute to a deeper understanding of mixed-spin quantum systems and may offer insights for future theoretical and experimental studies.

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Optical Insights into Spin-State Switching in Iron(II) Complexes

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This work presents a comprehensive investigation of the thermal and photoinduced spin-crossover (SCO) behavior of N-heterocyclic Fe(II) complexes $Fe(Me_2\text{-}3\text{-}bpp)_2(ClO_4)_2\cdot 2H_2O$ & $Fe(Me_2\text{-}3\text{-}bpp)_2(BF_4)_2\cdot 2H_2O$ (Me_2-3-bpp = 2,6-bis[5-methyl-1H-pyrazol-3-yl]pyridine) in hydrated and dehydrated KBr-dispersed forms. Thermal and light-induced spin transitions were studied in optically transparent KBr pellets and compared with reported powder magnetic data. Pelletization introduces mechanical strain and defects, influencing spin-state energetics ($\otimes E^0_{HL}$) and SCO cooperativity. The hydrate $Fe(Me_2\text{-}3\text{-}bpp)_2(ClO_4)_2\cdot 2H_2O$ exhibits a gradual and incomplete spin transition (~60% HS at 300 K), while the dehydrated form stabilizes the HS state (~76% HS at 5 K). The hydrated phase shows no LIESST effect due to a strong ligand field and LS stabilization. In contrast, the dehydrated form exhibits a clear LIESST response (T(LIESST) = 34 K) with stretched-exponential relaxation. For the $Fe(Me_2\text{-}3\text{-}bpp)_2(BF_4)_2\cdot 2H_2O$, hydration leads to a gradual and incomplete Spin transition (~40% HS at 300 K), while dehydration induces a complete spin transition and shifts spin transition temperature. Light-induced excited spin-state trapping (LIESST) studies further highlight remarkable phase-dependent behavior. The T(LIESST) value increases from ~30 K in the hydrated form to ~48 K in the dehydrated sample, underscoring the role of lattice dehydration, enhanced thermal trapping of the photoinduced HS state, consistent with increased lattice rigidity.

Keywords: *Spin-crossover, Zero-point energy difference, Cooperativity, Magnetism, Optical spectroscopy*

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Low-Temperature Cluster Spin-Glass State in Nickel Hexacyanoferrate

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Molecule-based magnets form a diverse family of organic, organometallic, and inorganic coordination compounds. Among these, porous bimetallic cyanide-bridged frameworks, commonly referred to as Prussian blue analogues (PBAs), $X_jA_k[B(CN)_6]$ (A, B = 3d transition metals; X = Li, Na, K, Cs, or Rb) have attracted considerable attention for their multifunctional properties. These include gas adsorption, photomagnetism, spin-crossover, magnetic pole inversion, and promising applications in batteries, supercapacitors, and sensor fabrication.

The nickel hexacyanoferrate framework compound, $Ni_{1.5}^{II}[Fe^{III}(CN)_6].nH_2O$ was synthesized via a simple co-precipitation method at room temperature. Structural characterization by room-temperature powder X-ray diffraction, followed by Rietveld refinement, confirmed a single, phase-pure crystalline phase with a face-cantered cubic structure (space group Fm-3m) and a lattice parameter of 10.21 Å. DC magnetization data show a transition from a paramagnetic to a ferromagnetic state at a Curie temperature of about 30 K. Fitting the susceptibility to the Curie–Weiss law yields a positive paramagnetic Curie temperature, confirming dominant ferromagnetic interactions. The effective paramagnetic moment, $\mu eff=3.4\mu_B$ per formula unit, agrees well with the spin-only calculated value of 4.07 μ_B/f.u. AC susceptibility provides additional insight into the magnetic dynamics. The frequency dependence of the susceptibility peaks was analyzed using the dynamic scaling power law. The extracted critical exponent product, $z\upsilon=5.06$, falls in the expected range for a cluster spin-glass system. This indicates that while DC magnetization suggests ferromagnetic-like ordering, the AC data reveal that the true low-temperature state is governed by the freezing of interacting magnetic clusters.

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Whispers of Coherence: Interfacing Molecular Dynamics and First-Principles Calculations to Understand Molecular Qubit Monolayers

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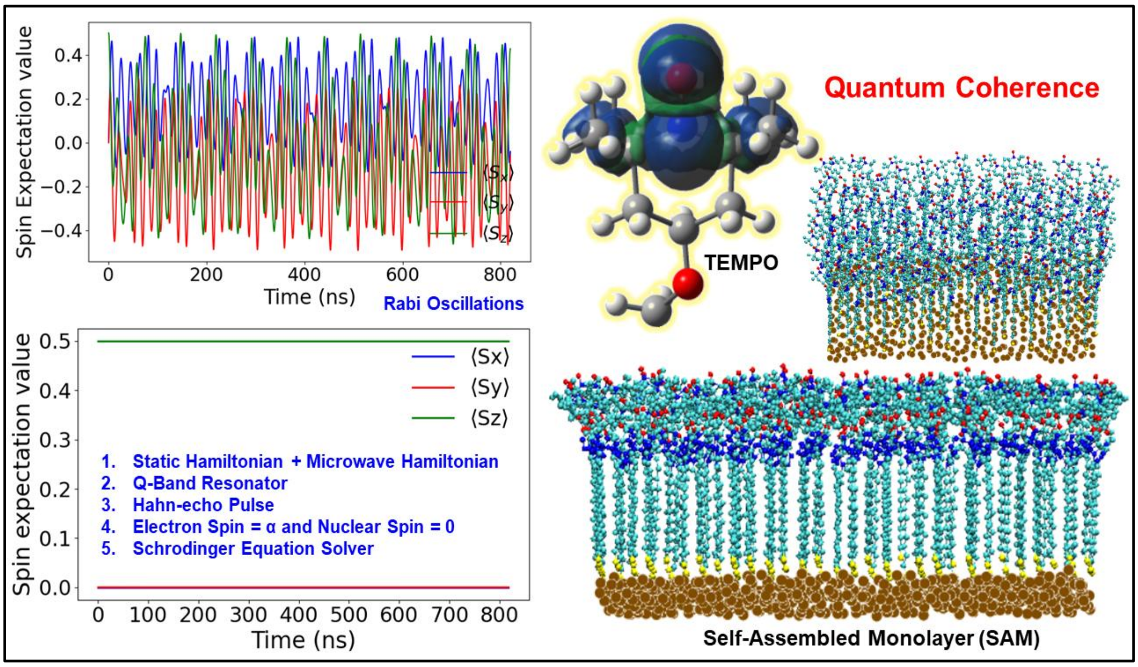
The pursuit of quantum technologies is fueled by the promise of exponentially faster computation. Among molecular spins, nitroxide radicals such as TEMPO have emerged as promising qubit candidates due to their long coherence times and chemical versatility. Recent study[1] shows that self-assembled monolayers (SAMs) of TEMPO radicals on Au(111) retain quantum coherence up to 13 μs. However, little is known about the spin dynamics in the qubits of the monolayers. We perform a comprehensive theoretical study to unravel the molecular origins of this behaviour. Using density functional theory (DFT) and *ab initio* molecular dynamics (AIMD), we first characterise the electronic structure, low-temperature vibrational modes, spin-phonon coupling, and longitudinal relaxation time (T_1) of an isolated TEMPO radical. We then extend our investigation to dimeric and trimeric TEMPO assemblies, determining spin-spin coupling, Zeeman and hyperfine tensors, and exploring their spin dynamics. Finally, we explore interfacial dynamics of TEMPO-based SAMs on Au(111) surface to understand how molecular motion and structural organisation at the interface dictate spin relaxation pathways.



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Anomalous magnetic anisotropy and effects of field cooling in a single 40 nm $\mathrm{Fe_3O_4}$ nanoparticle

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Magnetization ($\vec{\mathrm{m}}$) reversal in individual single magnetic nano-particles provides unambiguous information [1] which in bulk ensembles suffers from inter-particle interaction and averaging over particle size, shape, orientation, and defect configurations. A 40 nm size $\mathrm{Fe_3O_4}$ nano-particle was placed on the weak link of a Nb μ-SQUID for optimal coupling as shown in Fig. 1. The M-H measurements of this ferrimagnetic particle at 2 K show single domain characteristics**.** A model is discussed to understand how different components of $\vec{m}$ contribute to the magnetic flux through the SQUID loop. The experimentally determined angle dependent switching field is found to be close to that predicted by the generalised Stoner-Wohlfarth model, or the asteroid model, with a mixture of cubic and biaxial anisotropies [2].

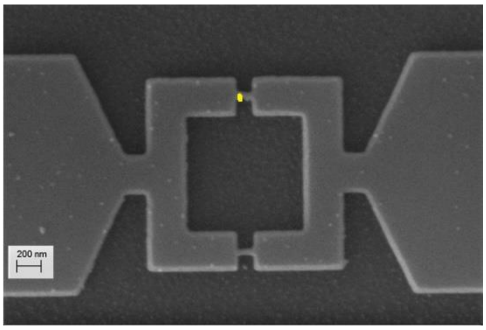

Figure 1: SEM image of 40 nm single $\mathrm{Fe_3O_4}$ nanoparticle (yellow colour dot) placed on the top weak link of the niobium μ-SQUID.

Due to the mixed anisotropy the angle dependent switching field exhibits multiple crossings at certain angles. The particle also exhibits changes in anisotropy in different cooling runs from room temperature and after ambient exposure. $\mathrm{Fe_3O_4}$ in bulk is known to exhibit a metal-insulator Verwey transition near 115 K with crystallographic change from an inverse spinel structure above 115 K and a monoclinic structure below it. Under this transition a slight change in c-axis lattice parameter can lead to a deformation and change in anisotropy. Our initial attempts to control the anisotropy-axes through field cooling failed with field-cooling from up to 200 K temperature and 1.6 T magnetic field. However, when it is cooled from above 375 K we see the anisotropy is cooling-field-direction dependent for cooling from above about 115 K. This is discussed in terms of water adsorbed on particle surface giving a surface strain which dominates the energetics over the field cooling leading to same distortion in every field cooling run from above 115 K despite presence of large fields. The field-cooling controlled anisotropy can have applications in nanotechnology and spintronics.

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Photocatalytic Degradation of Azithromycin Using CNC-TiO_2 Nanocomposites: A Sustainable Solution to Antibiotic Pollution and Resistance

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The widespread use of antibiotics, particularly during and after the COVID-19 pandemic, has increased antibiotic-resistant bacteria, raising significant concerns for public health and the environment[1]. One such pollutant, azithromycin (AZM), has been detected in high concentrations worldwide, underscoring the urgent need for effective removal strategies[2]. TiO_2 nanoparticles are recognized for their photocatalytic efficiency. However, they encounter practical challenges, such as difficulty in recovery, which can lead to secondary pollution[3]. Thus, it is essential to develop an appropriate substrate material or scaffold that can match the catalytic performance of these nanoparticles. This study explores the use of innovative cellulose nanocrystals (CNC) as a framework for creating composites with high-loading TiO_2 nanoparticles, offering a simple and efficient solution for the degradation of AZM. Characterization techniques, including FESEM, EDS, XRD, FT-IR, BET, UV-DRS, and UPS were utilized to confirm the structure and properties of the catalyst. Degradation experiments employed UV irradiation while optimizing catalyst dosage, pH, and reaction time. Under optimal conditions—using a 170 mg/L CNC-TiO_2 catalyst at pH 3 and exposing a 10 mg/L AZM solution to 125 W UV light for 180 minutes, above 99% degradation of AZM was achieved. Scavenger studies identified $O_2^{-\bullet}$ and •OH radicals as the primary active species. LC-MS/MS analysis also elucidated degradation pathways and intermediates, while toxicity studies indicated a reduction in harmful byproducts. The reusability of the catalyst was also demonstrated. This method presents a sustainable approach to treating AZM-contaminated waters, contributing to the mitigation of antibiotic resistance and environmental health protection.

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Cyano-bridged discrete heterometallic dimer and trimers: Synthesis, characterization and magnetic analysis

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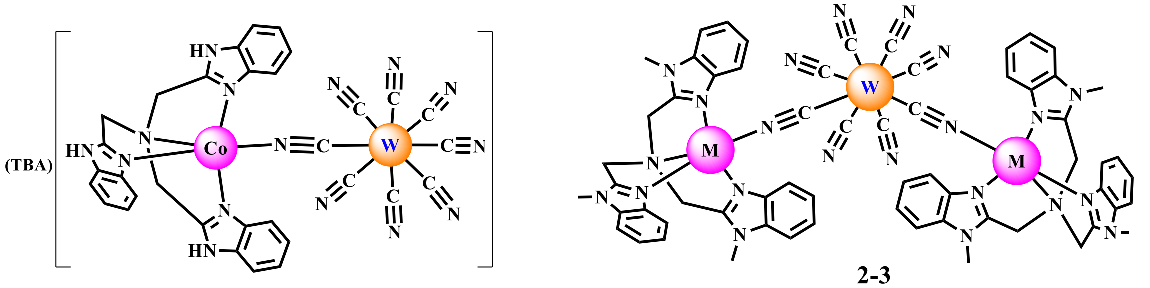
Engineering low dimensional molecular magnetic materials endowed with multifunctionality is currently experiencing renaissance of research interests due to their application in molecular data storage devices, sensors *etc*[1]. In this regard, cyanide bridged Prussian Blue Analogues (PBAs) show diverse physical properties such as high T_c ferrimagnetism, thermal phase transition, spin crossover *etc*[2,3]. In this work, one novel heterometallic dimer with molecular formula $(^{n}Bu_3NH)[Co^{II}(NTB)(\mu\text{-}CN)W^{V}(CN)_7]\cdot 3H_2O$ (**1**) and two trimer viz $[Co^{II}(Me_3NTB)(\mu\text{-}CN)_2W^{IV}(CN)_8]\cdot 10H_2O$ (**2**) and $[Fe^{II}(Me_3NTB)(\mu\text{-}CN)_2W^{IV}(CN)_8]\cdot 15H_2O$ (**3**) are synthesized. Single-crystal X-ray diffraction reveals formation of dumble shaped dimer in **1** (Co-W) and bent shaped in trimer in case of **2** (Co_2W) and **3** (Fe_2W). Co and Fe centers **1-3** are in trigonal bipyramidal geometry. Other Spectroscopic techniques, including FT-IR and UV–Vis and electrochemical analysis confirms the oxidation state of the metal centres involved. Magnetic investigations using variable-temperature DC and AC susceptibility measurements show significant exchange coupling between Co(II) and W(V) centers in **1**. Further presence of trigonal bipyramidal Co centers in **1** and **2** leads to the axial magnetic anisotropy (Scheme 1). On the other hand, two Fe(II) centers in **3** shows both positive and negative D value respectively.



1

1: M= Co, $J = 0.374\ cm^{-1}$, $D = -7.3\ cm^{-1}$

2-3

2: M= Co, $D_{Co1} = D_{Co1} = -8.1\ cm^{-1}$

3: M= Fe, $D_{Fe1} = 7.47\ cm^{-1}$, $D_{Fe2} = -13.5\ cm^{-1}$

Scheme 1: Schematic diagram of **1-3** with their exchange interaction and ZFS parameters.

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Engineering Molecular Bistability: Stimuli-Driven Spin-State Switching in Metallosupramolecular Systems

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The practical integration of molecular magnetic materials into electronics and quantum technologies critically depends on their ability to exhibit bistability, typically realized through reversible transitions between high-spin (HS) and low-spin (LS) states of 3d metal ions under external (light, temperature, pressure) or chemical (pH, redox) stimuli.[1] Nature-inspired self-assembly via metal–ligand coordination offers a powerful platform to construct metallosupramolecular architectures, where strong cooperativity between metal centers drives bistable molecular systems.[2] Such discrete complexes are increasingly recognized as multifunctional systems with potential in sensing, gas separation, catalysis, and biotechnology.[3] Our work advances this field by pursuing the rational design of 3d metal-based supramolecular assemblies to realize a spectrum of stimuli-responsive functions, including photoluminescence,[4] spin-crossover phenomena,[5] and single-molecule magnetism (SMM).[6]

In this presentation, I will highlight three distinct systems: (i) a Co(II)-based tetrahedral cage that uniquely combines spin-state switching with SMM behavior, (ii) tetranuclear [2×2] Fe(II) grids that undergo pH-responsive spin-state switching both in solid state and in solution, and (iii) dinuclear Fe(II) helicates that display thermo-induced spin-state modulation governed by ligand field strength, coupled with striking photomagnetic properties. Together, these systems demonstrate how targeted molecular design can unlock multifunctionality in switchable magnetic materials, providing design principles directly relevant to future molecular electronics and information technologies.

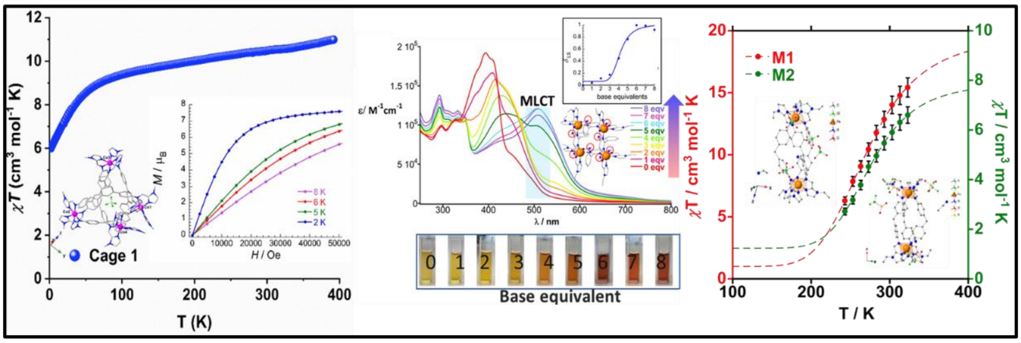

Figure: SCXRD structures of cage, grid, and helicate complexes, linking topology to switchable magnetic and electronic properties.

Acknowledgement: We gratefully acknowledge the Indian Institute of Science (IISc), the Solid State and Structural Chemistry Unit (SSCU), the Department of Science and Technology (DST), the DST-Nano Mission (DST, Project No. DST/NM/TUE/QM-10/2019(G)/1), Anusandhan National Research Foundation (ANRF-SERB, Core Research Grant CRG/2023/003081), and the Indo-French Centre for the Promotion of Advanced Research (CEFIPRA / Centre Franco-Indien pour la Promotion de la Recherche Avancée, CSRP Project 70T07-2) and Prime Minister's Research Fellowship, Ministry of Education, Government of India for their generous funding support.

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Spin-Vibrational Relaxation in Cr(V) and V(IV) Tetraphenyl Porphyrin Molecular Spin Qubit Candidates

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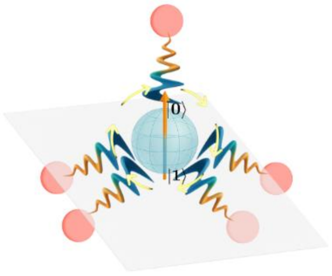
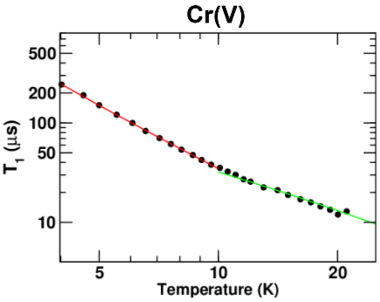
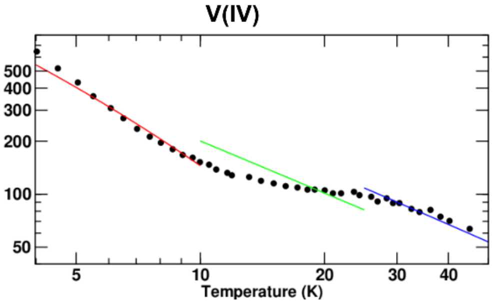
The second quantum revolution has introduced the potential of quantum systems for applications in sensing, communication, and computation, with molecules emerging as promising candidates due to their tunability and specificity. However, achieving room-temperature electron spin coherence in molecular qubits remains a major challenge, as high-temperature coherence is often limited by the spin-lattice relaxation time T_1. We report a detailed computational study on the magneto-structural factors underlying in the spin-lattice relaxation of two transition metal-based molecular spin qubit candidates, V(O)TPP and Cr(N)TPP (TPP = tetraphenyl porphyrin), using density functional theory, multi-configurational ab initio methods, and spin-vibration coupling models. The ab initio calculated spin-vibrational coupling coefficients for low-frequency modes are applied within a perturbative spin-vibrational relaxation framework to estimate T_1 relaxation times and their anisotropy. The faster T_1 relaxation in Cr(V) is attributed to the low-frequency ligand breathing modes, while the pronounced T_1 anisotropy in V(IV) is reflective of its electronic structure and angular momentum coupling pathways. The model reveals how vibrational and electronic factors govern spin relaxation. The anisotropy in T_1 relaxation is found to arise from specific metal-ligand vibrations that are strongly coupled to certain orbital-specific ligand field states. These insights are hoped to advance the rational design of transition metal-based qubits with improved coherence and relaxation characteristics.







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Probing the Structure-Conductance-Bias Relationship in Atomic-Scale Metallic Junctions

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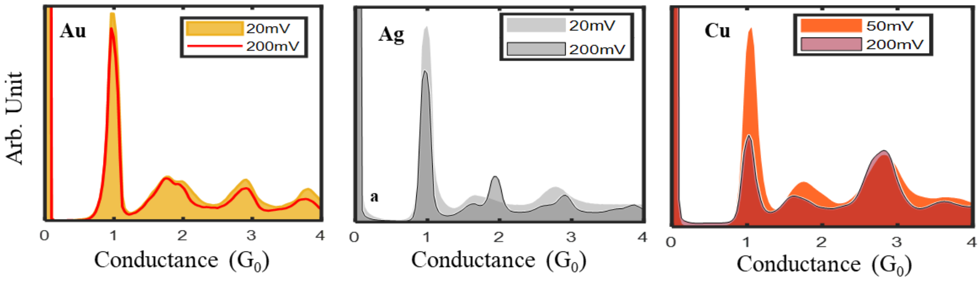
Advancing nanoscale electronic devices requires a fundamental understanding of how atomic-scale geometry governs charge transport in metallic junctions. The conductance behavior of such systems is not determined solely by the electronic structure of the constituent metal but also by the precise geometric configuration of the junction at the atomic level. Even subtle rearrangements of atoms can lead to substantial changes in the number and transmission probability of conductance channels.

In this work, we explore the correlation between metal junction geometry and conductance in different metallic systems-Au, Ag, and Cu-formed using the mechanically controlled break junction (MCBJ) technique. By systematically varying electrode separation, we achieve atomic contacts with well-defined configurations and analyze conductance quantization as a function of geometry. Conductance histograms and two-dimensional correlation analyses reveal distinct signatures corresponding to single-atom contacts, dimer formations, and chain-like structures. Moreover, bias-dependent conductance measurements show clear evolution of histogram features and stability regimes, reflecting the combined influence of local heating, atomic rearrangement, and bias-induced modification of the electronic structure.

Our findings highlight the critical role of atomic geometry in determining conductance evolution and bias response in metallic junctions. This structure–conductance–bias relationship provides important insights into the microscopic mechanisms governing electron transport, serving as a foundation for designing stable, reproducible atomic and molecular junctions for future nanoscale electronic and quantum device applications.



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Effect of salts and electric field perturbations on the internal droplet dynamics of bio-colloidal solutions

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The evaporation-driven pattern formation in bio-colloidal sessile droplets has gained significant attention for its relevance in disease diagnostics, biosensing, and healthcare applications. While prior studies have explored the evaporation dynamics of individual components such as salts, micro-sized colloidal particles, and protein-laden fluids, the coupled influence of salts and externally applied electric fields on desiccation patterns remains largely unexplored. In this study, we systematically examine the role of salt-mediated electrical double layer (EDL) interactions in colloidal suspensions, using droplet desiccation as a model phenomenon, and extend our investigations to electrowetting-on-dielectric (EWOD) platforms to assess the influence of applied electric fields on evaporation and deposit morphology.

Our experiments reveal three key regimes: (i) At high salt-to-particle concentration ratios, an initial constant contact radius (CCR) mode transitions to a constant contact angle (CCA) mode, leading to large grid-like salt crystallites with single nucleation sites. As evaporation progresses, inward Marangoni recirculation drives colloidal particles toward the crystal interfaces, forming centralized depositions and subsequently orthoradial cracks emanating from the compaction band. (ii) As the particle concentration decreases, the compaction band width and crack density are significantly reduced, with fewer stress-relieving fractures. (iii) At sufficiently low colloidal loading, crack-free deposits are observed across all salt concentrations. These findings are further analysed under EWOD conditions, where an applied electric field significantly modulates droplet evaporation dynamics, desiccation morphologies, and salt crystallization kinetics. This study provides a quantitative physicochemical framework for understanding salt-induced colloidal interactions and electric-field-assisted drying, with potential applications in biosensing, microfluidics, and lab-on-a-chip technologies.

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Generalized Heisenberg-Type Magnetic Phenomena in Coordination Polymers with Nickel−Lanthanide Dinuclear Units

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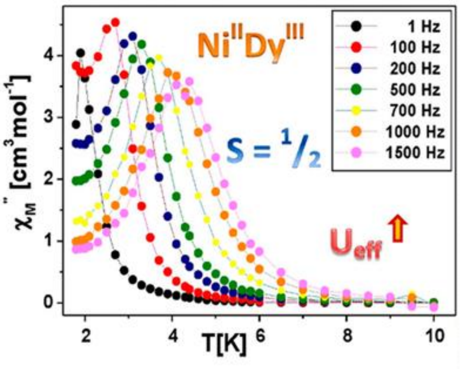
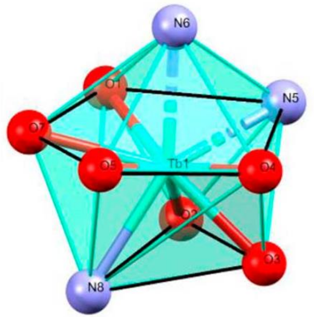
A new family of 3d−4f coordination polymers with the molecular formula $[Ni^{II}Ln^{III}(L)(dca)_2(NO_3)]_n$ [Ln = Eu (**1**), Gd (**2**), Tb (**3**), Dy (**4**), and Ho (**5**); H_2L = N,N′-bis(2-hydroxy-3-methoxy-5-methylbenzyl) homopiperazine; dca = dicyanamide] has been synthesized in search for new single-molecule magnet (SMM) materials containing highly anisotropic lanthanides. The magnetic properties of these materials have been established by DC and AC magnetometry and explained quantitatively by comprehensive phenomenological modeling based on a generalized Heisenberg-type model, hypothesized previously based on first-principles calculations. Single-crystal X-ray diffraction has shown that the compounds are isostructural, with lanthanide atoms occupying a nine-coordination site with muffin-like geometry and individual NiII−LnIII units linked by dca anions. Other than the paramagnetic compound **1**, **2−5** exhibit intraunit ferromagnetic 3*d*−4*f* interactions, favorable for a large spin ground state. A slow field-induced relaxation of magnetization has been observed in compound 4 (only), displaying a substantial energy barrier of U_{eff}/k_B = 26.2(5) K, below 6 K. This is attributed to an easy-plane anisotropy and is consistent with the relaxation in systems with a Kramers ground state doublet and hyperfine interactions.





Muffin-like geometry around the Tb

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Modeling of a one-dimensional atomic-scale carbon strip decorated with transition metal adatoms for Magnonic applications

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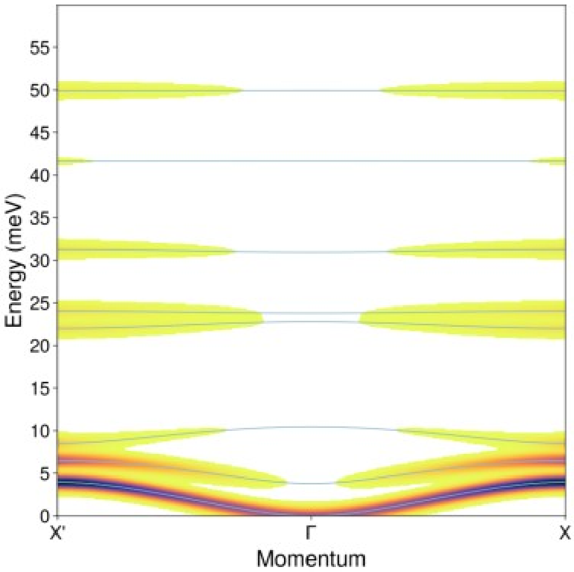
The present work reports the modeling of one-dimensional atomic-scale carbon strip decorated with transition metal adatoms. The electronic structure is investigated by using Density Functional Theory (DFT). By transforming plane-wave solutions into Wannier orbitals and employing the magnetic force theorem, the exchange interactions within the system are determined[1]. The resulting magnetic structure is analyzed, revealing terahertz-frequency acoustic and optical magnonic bands[2]. The presence of these bands, along with their tunability under external magnetic fields, highlights the potential of this system as a promising platform for magnonic applications[3]. Figure: The magnon dispersion spectra for the carbon strip with Mn adatom along the path X'-Gamma-X.



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Cyanido bridged {Fe_2Ni_2} molecular squares

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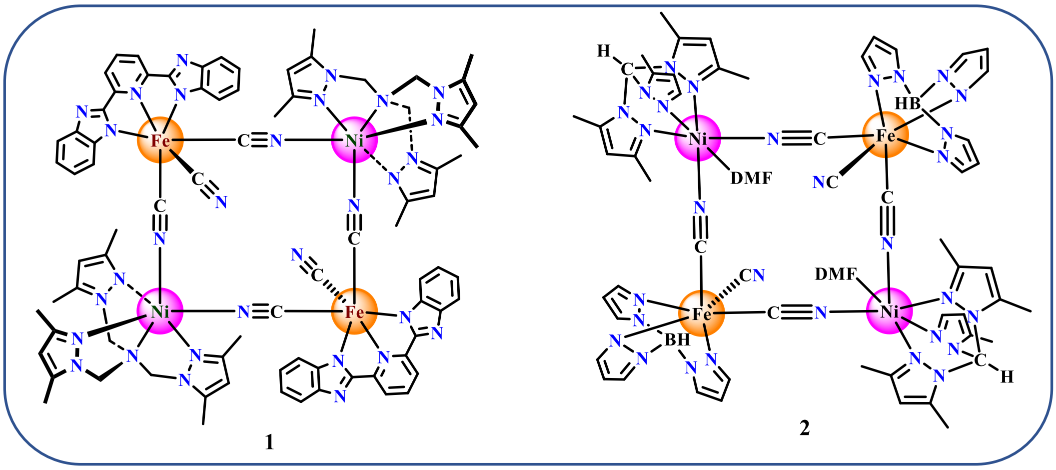
Cyanido-bridged heterometallic assemblies have long served as ideal model systems for exploring metal-to-metal charge transfer (MMCT) and magnetic exchange coupling. In this work, we report the synthesis of a molecular square complex, $[\{Ni(TPA)(\mu_2\text{-}NC)_2Fe(bbp)(CN)\}_2]\cdot 10H_2O$ (**1**), featuring a $[Fe_2Ni_2]$ core. Furthermore, a new analogue with the same $[Fe_2Ni_2]$ core, but incorporating facial-tricyanidometallate and *N*-donor ligands at the Ni site, has been synthesized with the formula $[\{Ni(TPM)(\mu\text{-}NC)Fe(Tp)(CN)_2(DMF)\}\{ClO_4\}]_2\cdot H_2O$ (**2**). Complex **2** exhibits remarkable single-molecule magnet (SMM) behaviour, as evidenced by frequency-dependent out-of-phase AC magnetic susceptibility signals. Comprehensive structural, spectroscopic, and magnetic investigations reveal that subtle electronic modulation within the cyanio-bridged framework of **2** enhances magnetic anisotropy. This study demonstrates a rational design strategy for developing cyanido-bridged molecular systems, advancing the field of molecular magnetic materials.



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“Electric field driven conformational modifications in metal-molecule-metal junction”

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Development of next-generation organic electronic devices depends on understanding of charge transport at single molecular level. Single-molecule junctions, consisting of individual molecules sandwiched between two electrodes, are commonly used in charge transport studies. During the past few decades, rapid technical and theoretical advances have improved our understanding of charge transport phenomena and different physical properties at the atomistic limit. Importantly, in recent times, there has been a great interest in combining single-molecule junctions with different control systems to study and optimize the important physical phenomena, including planarization, folding, trans-to-cis isomerization, and so forth. Our work focuses on how electric fields affect the conformation of the molecule and consequently its impact on the charge transfer to or from the molecule.

Here we show that conformation of the benzidine molecular junction can be greatly tuned by modifying bias voltage, and this junction can have two distinct conductance states with conductance values either high or low. While high conductance states become more dominant with the rise of bias voltage. The effect is opposite for the low-conducting state. Further experiment with benzene-1,4-diamine and 4,4'-(ethyne-1,2-diyl)dianiline molecular junctions reveals no such effect. Thus, our findings demonstrate that applied bias voltage is a key factor in realizing the desirable configuration of the benzidine molecular junction. Increase in bias voltage leads to change in the dihedral angle between two phenyl rings of benzidine molecule, which might be reflected in bias-sensitive molecular conformation. Theoretical MD simulation and transport calculation also support our observation. Overall, important role of the electric field in nano electromechanics is identified through our study, which enriches our knowledge for future generation nano-electronics applications.

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From Magnetic Exchange to Catalytic Efficacy: Unveiling Cyanide-Bridged Co-Fe Dimers with Five-Coordinated Co (II) Centre

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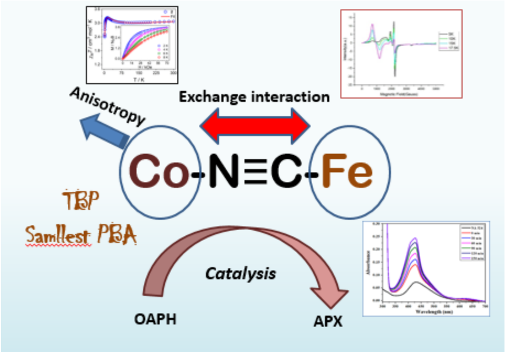
Cyanide-bridged heterometallic complexes continue to attract considerable attention owing to their diverse structural motifs and intriguing magnetic and catalytic properties. In this work, cyano-bridged [CoFe] molecular dimers featuring coordinatively unsaturated trigonal bipyramidal (TBP) cobalt(II) centers have been successfully assembled. The use of facial *N*-donor tetradentate ligands in combination with the tricyanometalate linker $[Fe(Tp^*)(CN)_3]^-$ [Tp* = hydrotris(3,5-dimethylpyrazol-1-yl)borate] led to the formation of two heterobimetallic cyano-bridged dimers: $[\{Co(Me_2TPA)(\mu\text{-}NC)Fe(Tp^*)(CN)_2\}][Fe(Tp^*)(CN)_3]\cdot 4.5H_2O$ (**1**) and $\{Co(NTB)(\mu\text{-}NC)Fe(Tp^*)(CN)_2\}\cdot 3H_2O\cdot CH_3OH$ (**2**). Structural analyses reveal that cyanide bridges core molecular structure with TBP Co(II) and low-spin Fe(III) centers. The nature of magnetic exchange interactions in these systems was investigated using DC magnetic properties and variable-temperature electron paramagnetic resonance (EPR) measurements, which provide evidence for ferromagnetic coupling between paramagnetic centers. Moreover, both complexes exhibit significant catalytic activity toward the oxidation of *o*-aminophenol to 2-aminophenoxazin-3-one, thereby functioning as efficient synthetic models for the enzyme phenoxazinone synthase. These findings highlight the interplay between structure, magnetism, and catalysis in cyano-bridged Co-Fe assemblies.



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Electronic and magnetic phases of a bipartite square-lattice in an extended Hubbard model

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Abstract

Transition metal oxides are interesting not only due to the presence of strongly electron correlations, but also due to the intricate interplay between charge, spin, orbital and lattice degrees of freedom. The competing nature of these interactions rise to novel and exotic electronic and magnetic ground states like the colossal magnetoresistance, superconductivity and non-trivial topological behavior to name a few. This study pertains to the investigations on the coupling between the spin and charge degrees of freedom in a two sub-lattice model. We employ an extended Hubbard model that incorporates site energy, on-site and inter-site Coulomb interactions, as well as the Hund's direct exchange. The model is solved using a mean-field approach to understand various electronic and magnetic ground states of the model by varying the model parameters. The phase diagram of the model obtained in various parametric planes reveal exotic phases like the charge-ordered antiferromagnetic (CO+AFM) phases, non-charge-ordered magnetic phases besides a fully charge-ordered phase. It will be shown that the CO+AFM (AM) phase is in fact an antiferromagnetic phase in which the Kramer's degeneracy is lifted in the momentum space, akin to the Rashba effect but in the absence of spin-orbit interactions. The projected band structure analysis further reveal that the altermagnetism originates from the strong coupling between the charge and spin degrees of freedom of the A- and B-sites. The various electronic and magnetic phases of the model will be described using the site spin and charge densities as well as the electronic band structures. This work thus presents a tunable framework for engineering novel altermagnetic materials.

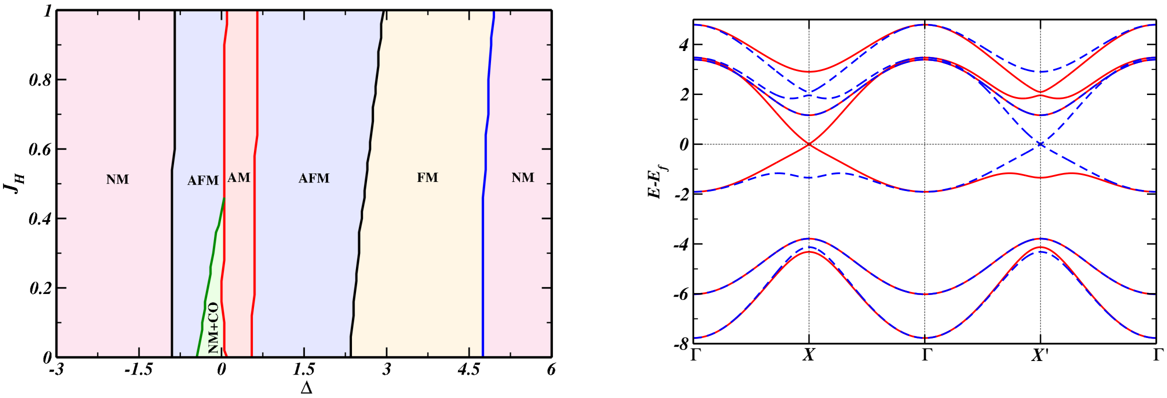

Fig-1: (Left) Phase diagram of a bipartite lattice in the J_H vs. Δ plane of the extended Hubbard model, where J_H represents the Hund's direct exchange and Δ is the site energy difference between the A and B sublattice sites. (Right) Energy band diagram of the CO+AFM (AM) phase for $J_H = 0.1$ and $\Delta = 0.2$. The up and down electron bands are shown as solid-red and dashed-blue lines respectively. The up- and down-spin bands are split in the momentum space along the $X - \Gamma - X'$ direction.

Keywords : Altermagnetism; extended Hubbard model; mean-field approach.

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Basis Adaptive Algorithm for Quantum Many Body Systems on Quantum Computers

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A new basis adaptive algorithm for hybrid quantum-classical platforms is introduced to efficiently find the ground-state properties of quantum many-body systems. The method addresses limitations of many algorithm like VQE and QPE etc by using shallow Trotterized circuits for short real-time evolution on a quantum processor. The sampled basis is then symmetry-filtered by using various symmetries of the Hamiltonian which is then classically diagonalized in the reduced Hilbert space. We benchmark this approach on the spin-1/2 XXZ chain up to 24 qubits using the IBM Heron processor. The algorithm achieves sub-percent accuracy in ground-state energies across various anisotropy regimes. Crucially, it outperforms the Sampling Krylov Quantum Diagonalization (SKQD) method, demonstrating a substantially lower energy error for comparable reduced-space dimensions. This work validates symmetry-filtered, real-time sampling as a robust and efficient path Basis Adaptive Algorithm for Quantum Many-Body Systems on Quantum Computers for studying correlated quantum systems on current NISQ hardware.

Dynamic Molecular Systems: Electron, Spin, and Valence State Modulation

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The design and synthesis of switchable molecular materials hold great promise for advancing molecular electronics, data storage, and sensing technologies by enabling functional miniaturization. Such systems exploit external stimuli such as temperature, pressure, or light to access photomagnetic phenomena and bistability near room temperature.[1] More than 25 years of successful cyanide-based chemistry have led to synthesizing an array of cyanide-bridged polymetallic systems based on a building block approach that exhibits significant importance in molecular magnetism.[2] Amongst them, a particular interest has been given to various molecular model complexes of mixed-valence [FeFe] Prussian Blue (PB) and [FeCo] Prussian Blue Analogues (PBAs), e.g., molecular cubes, squares, and dinuclear units.[3] Alongside these cyanido-based systems, cobalt–dioxolene complexes undergoing valence tautomerism provide another powerful platform for probing dynamic electronic rearrangements.[4]

In this work, I will present a comparative study of three representative systems: (i) Fe–Co molecular assemblies exhibiting metal-to-metal electron transfer (MMET) driven bistability[5], (ii) alkali-ion inserted Fe_8 cubes displaying spin crossover (SCO) behaviour, and (iii) cobalt–dioxolane complexes undergoing valence tautomerism (VT). Together, these systems highlight versatile pathways for achieving dynamic modulation of electronic, spin, and valence states, underscoring the potential of molecular design in tailoring multifunctional switchable materials.

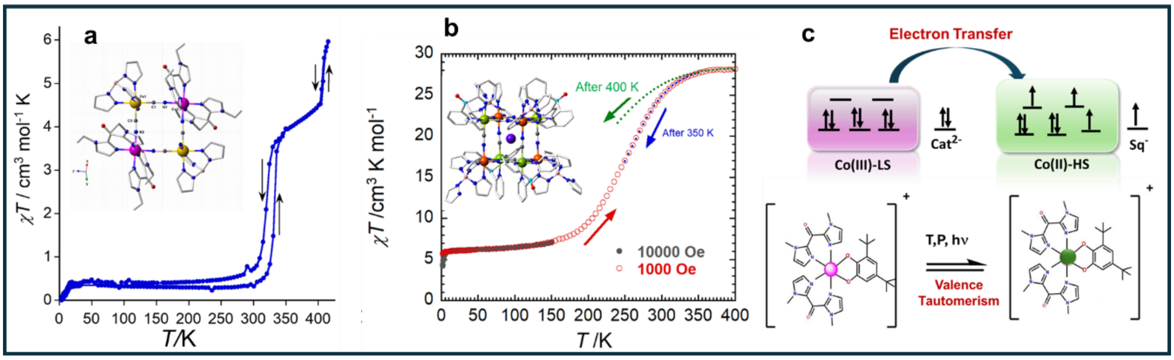

Figure: Perspective view of Fe_2Co_2 molecular square undergoing thermo-induced MMET **(a)**, Reversible thermo-induced Spin State Switching in Alkali-inserted Fe_8 cube (**b**), and Electron transfer mechanism of cobalt–dioxolane Valence tautomeric system (**c**).

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Room-Temperature Near-Infrared Excitons and Optoelectronics in 2D/Organic Heterostructures via Spontaneous Epitaxial Growth

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Two-dimensional (2D) materials, with their atomic-scale thickness and extraordinary physical properties, have become a cornerstone of modern materials research, offering exciting possibilities for future nanoelectronics and optoelectronic devices. Introducing organic molecules onto 2D surfaces enables the creation of hybrid interfaces where charge transfer, molecular orientation, and interfacial interactions can be precisely tuned to manipulate the material's electronic and optical behaviour. In this work, we demonstrate that vanadyl phthalocyanine (VOPc) molecules can self-assemble into highly ordered ultrathin films on atomically flat van der Waals crystals such as MoS_2, WS_2, graphene, and hBN under ambient conditions. The resulting heterostructures exhibit a pronounced photoluminescence (PL) blue shift—from 870 nm to 805 nm—arising from dipole-mediated molecular dimer formation. Comprehensive studies of VOPc/MoS_2 hybrid interfaces uncover pronounced interfacial charge-transfer processes that give rise to mixed or hybrid excitonic states, as revealed by transient absorption spectroscopy. Complementary insights from X-ray Photoelectron Spectroscopy (XPS), Ultraviolet Photoelectron Spectroscopy (UPS), and UV-Vis Spectroscopy collectively confirm the emergence of a coupled 2D/organic electronic structure that promotes the stabilization of bound excitons across the interface.

Importantly, when incorporated into a phototransistor architecture, the VOPc/MoS_2 hybrid channel exhibits highly enhanced photo response, achieving a responsivity on the order of 10^5 A W^{-1} under 810 nm LED illumination. This exceptional performance highlights the synergistic role of molecular ordering, interfacial dipoles, and hybrid exciton formation in amplifying photocarrier generation and transport. Together, these results demonstrate that molecular arrangement and local structural ordering can be strategically leveraged to tune both the optical response and device functionality of 2D/organic heterostructures—particularly within the near-infrared regime—while providing a versatile platform for exploring unconventional excitonic phenomena and spin–valley interactions in hybrid quantum materials.

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