

# Programme Booklet

**MODERN TRENDS IN MOLECULAR MAGNETISM  
(MTMM- IV)**

**&**

**SPINS IN MOLECULAR SYSTEMS:  
EXPERIMENT, THEORY AND APPLICATIONS  
(SiMS - III)**

**5<sup>th</sup> - 8<sup>th</sup> November 2024**

**Venue: AVR Auditorium & RBM Lecture Hall  
Solid State and Structural Chemistry Unit  
Chemical Sciences Division  
Indian Institute of Science, Bengaluru**



**Organized by Team M2S**



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## Conveners

Prof. Abhishek Mondal

Prof. S. Ramasesha

## Local Organizing Committee

Dr. Awadhesh Narayan

Dr. Bhagwati Prasad,

Dr. Soumen Ghosh

Dr. Sujit Das

Dr. Susanta Hazra

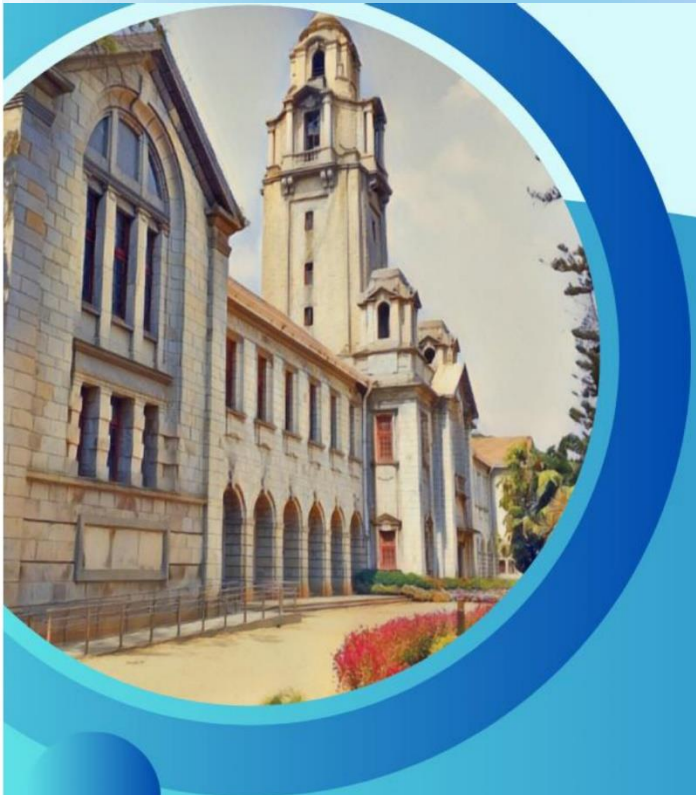
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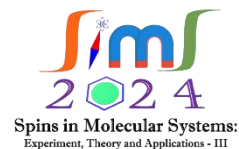


## Other





A Warm Welcome to  
Indian Institute of Science



The Solid State and Structural Chemistry Unit (SSCU), Indian Institute of Science, Bangalore, India, on behalf of entire scientific fraternity of IISc, welcomes you all to the **Indian Institute of Science, Bangalore (IISc)**.

We are buoyant to host the International Conference on **Modern Trends in Molecular Magnetism – IV (MTMM – IV)** & **Spins in Molecular Systems: Experiment, Theory and Applications - III, SiMS-2022 (SiMS – III)** (<https://mtmm-sims2024.in/>). The entire Solid State and Structural Chemistry Unit is privileged to welcome you all to the marvelously beautiful campus of IISc (<https://www.iisc.ac.in/>), which is truly the first example of a public-private partnership in this country; an institution whose evolution over a century is testimony to the robustness of its foundations. The campus amasses classical architecture, harboring exotic and indigenous plant species with about 150 species of woody plants and various people from different parts of India and abroad. The institute has housed many eminent scientists, including Sir C. V. Raman, Prof. G. N. Ramachandran, Prof. Satish Dhawan, and Prof. C. N. R. Rao. The institute is a blend of devoted faculty and motivated students working together and contributing to society since 1909.

**MTMM – IV & SiMS – III** have a lot to offer to all who came to enjoy the blend of excellent science and joyful fellowships on a breathtaking campus. The conference houses many eminent scientists from across the globe, where a plethora of knowledge and information will be exchanged on the various theoretical and applicative aspects of **Magnetism**. The conference will act as a platform to help in integrating chemists, physicists, and materials scientists from different fields of theory and experimentation, where advancement in **Switchable Magnetic Materials, Single -Molecule Magnets, Spin-State Switching, Photomagnetism and Luminescent Systems, Magnetism in Nanomaterials and 2D Materials, New Generation Quantum Materials, Spin Liquid Systems, Spintronics and Quantum Computing, Organometallic and F-Element Chemistry, Magnetism in MOF/COF Systems, Magnetism in Supramolecular Systems (Molecular Clusters and Coordination Cages), Spins in Biological Systems, Advanced Synchrotron Techniques: EPR (High Magnetic Field and Pulse EPR) & NMR, Advanced Quantum Chemical Calculation** will be discussed. The collective interaction of physics and chemistry will enhance the field in a great and healthy atmosphere.

**The Organizing Committee is pleased to welcome you aboard the Modern Trends in Molecular Magnetism – IV & Spins in Molecular Systems: Experiment, Theory and Applications – III.**

### Organizing Committee Conveners

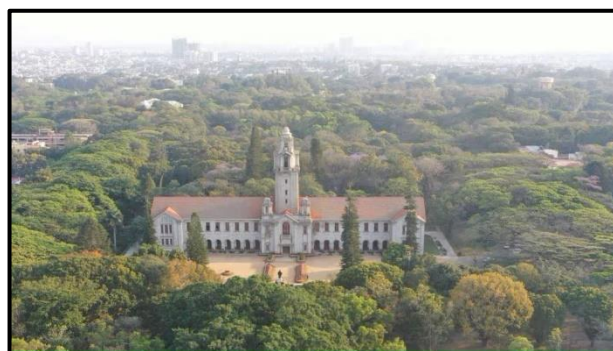
**Prof. Abhishek Mondal & Prof. S. Ramasesha**



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## How to REACH IISc

Bangalore is well connected by Air, Rail, and Road to all the metropolises and most major cities of the country. Now you can fly direct to Bangalore from several international airports as well. The Institute is also known as “Tata Institute” to the locals. It is better to use the name “Tata Institute” with the taxi, auto-rickshaw drivers, and bus conductors. The institute is located between Malleswaram and Yeswantpura.



### Reaching IISc from the Airport:

IISc is about 35 kms from the airport. One could take a prepaid taxi (currently, costs about INR. 900, and the counter is available near the exit of the Airport Building), or a city taxi (costs about INR. 800, and a queue for the same is just outside the airport building). Also, one can book cab from Uber, Ola, Rapido apps (costs about INR. 800 depends on the availability and timing). The Institute is known as “Tata Institute” to the locals and is just past Mekhri circle and on the way to Yeshwantpura (one must take a right turn at Mekhri circle).

A Shuttle bus service, operated by **Airport Vayu vajra Services**, runs from the airport to various areas in Bengaluru city every 15-20 minutes. Details of the schedule can be found here (<https://mybmtc.karnataka.gov.in/new-page/Airport%20Vayu%20vajra%20Services/en>).

*Additional information on the airport can also be found at its official website: (<http://www.bengaluruairport.com/>).*

### Reaching IISc from SMVT Railway Station:

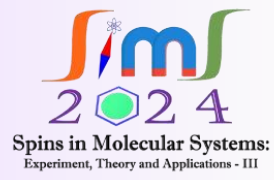
This is a relatively new railway station, located about 10 km away from IISc. The cost for Ola/Uber/Rapido Taxi/Auto ranges in INR 300-400.

### Reaching IISc from City Railway Station:

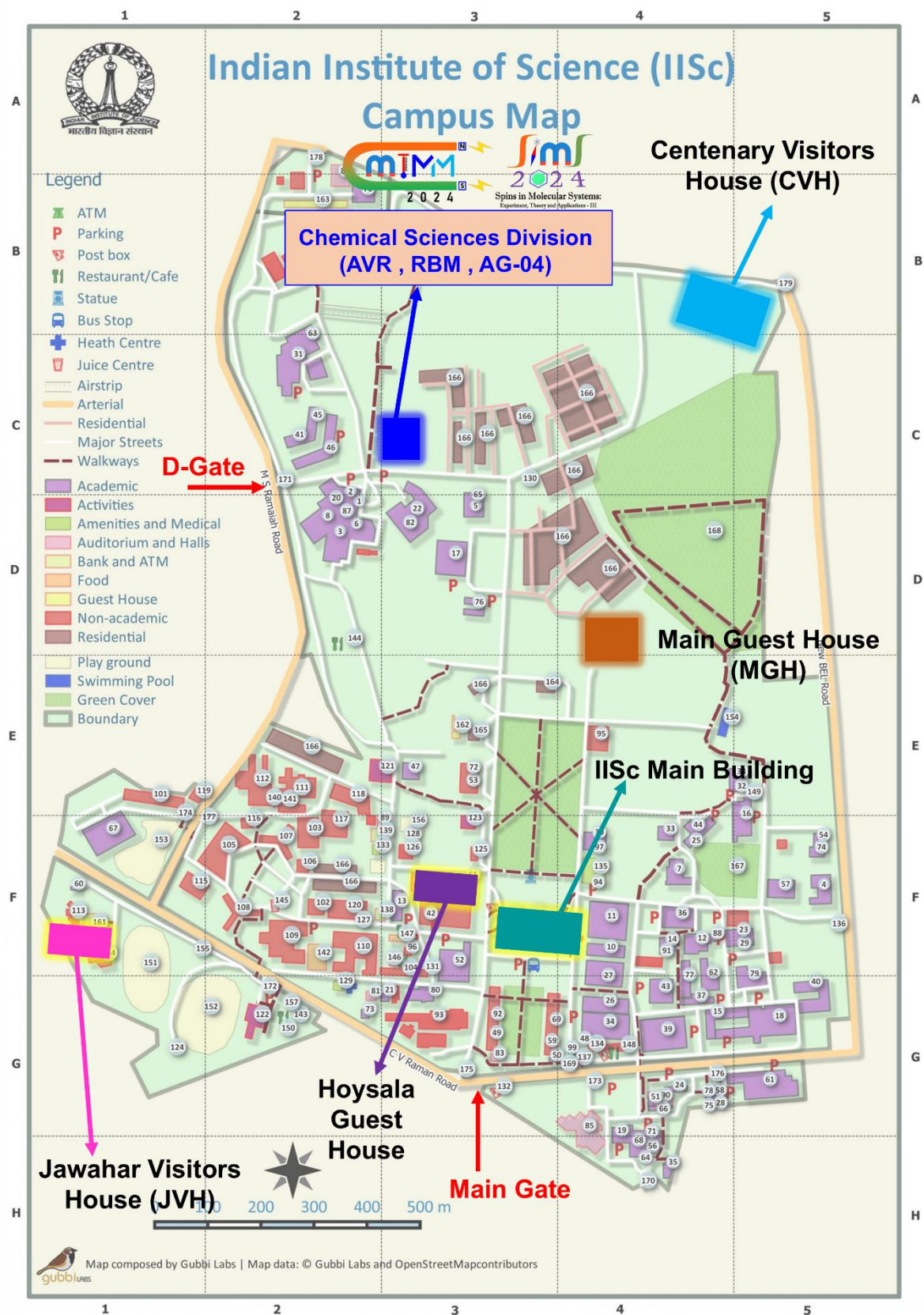
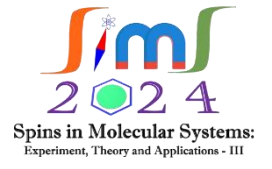
The City railway station is about 7 kms from the IISc campus. One will have to leave the station from platform number ONE and reach the prepaid taxi stand and hire a city taxi (costs about INR 250). Majestic (7kms from IISc) is the central Bus stand in Bengaluru and is just opposite the City Railway station. If one happens to reach Majestic, Bengaluru by bus, go to city bus platform number 22 from where almost all city buses come to the Institute.

### Bus stops near IISc:

If you go to the city and wish to take a bus back to IISc, you will have to move past Malleswaram 18th cross bus stand towards Yeshwantpura to return back to IISc. There is also a bus stop on the highway between the yellow over bridge and Prof. CNR Rao Circle, and another one is at Prof. CNR Rao circle (on Sir CV Raman Road). Finally, there is a bus stop at Yeshwantpura tollgate (more convenient while going from IISc), just off campus near R block. Most buses go to one of these places.



## Conference related Locations



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**MODERN TRENDS IN MOLECULAR MAGNETISM – IV**  
**&**  
**SPINS IN MOLECULAR SYSTEMS:**  
**EXPERIMENT, THEORY AND APPLICATIONS – III**



**SEARCH BY GROUPS AND SERIAL NUMBERS**

**Academics**

**Division of Biological Sciences**

Division of Biological Sciences .....	D2.....	1
Biochemistry .....	D2.....	2
Centre for Ecological Sciences .....	D2.....	3
Centre for Infectious Disease and Biosafety Lab .....	F5.....	4
Centre for Neuro Sciences .....	D3.....	5
Microbiology & Cell Biology .....	D2.....	6
Molecular Biophysics .....	F4.....	7
Molecular Reproduction, Development & Genetics .....	D2.....	8

**Division of Chemical Sciences**

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Materials Research Centre .....	F4.....	12
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**Division of Electrical Sciences**

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**Division of Interdisciplinary Research**

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## Google Map Navigations



- ❖ **Conference Venue: AVR Auditorium (A – Block, 2<sup>nd</sup> Floor, Chemical Sciences Division)**

[https://www.google.com/maps/place/A+V+Rama+Rao+Auditorium/@13.0254851,77.5540969,15z/data=!4m6!3m5!1s0x3bae170072e0ac2d:0xa11507858c340e41!8m2!3d13.0254843!4d77.5643961!16s%2Fg%2F11y6kc54!x?authuser=0&entry=ttu&g\\_ep=EgoyMDI0MTAyNy4wIKXMDSoASAFQAw%3D%3D](https://www.google.com/maps/place/A+V+Rama+Rao+Auditorium/@13.0254851,77.5540969,15z/data=!4m6!3m5!1s0x3bae170072e0ac2d:0xa11507858c340e41!8m2!3d13.0254843!4d77.5643961!16s%2Fg%2F11y6kc54!x?authuser=0&entry=ttu&g_ep=EgoyMDI0MTAyNy4wIKXMDSoASAFQAw%3D%3D)

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- ❖ **Hoysala Guest House (Beside Centre for Cryogenic Technology):**

<https://www.google.com/maps/dir//centre+for+cryogenic+technology/@13.01951,77.5650765,16z/data=!4m8!4m7!1m0!1m5!1m1!1s0x3bae17d683a1fb91:0x456be3ea189a2674!2m2!1d77.5655528!2d13.0169841?hl=>

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- ❖ **Jawahar Visitors House (JVH):**

<https://www.google.co.in/maps/dir//Indian+Institute+Of+Science,+Malleshwaram+Jawahar+Guest+House,+CV+Raman+Rd,+IISc+Gymnasium,+Malleshwaram,+Bengaluru,+Karnataka+560012/@13.0173341,77.5574501,15z/data=!4m8!4m7!1m0!1m5!1m1!1s0x3bae3d7dd13541e3:0xdf61dc0d4e73ce24!2m2!1d77.5595686!2d13.0167639>

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- ❖ **Centenary Visitors House (CVH):**

<https://www.google.com/maps/dir/13.0226894,77.5734042/iisc+CVH+guest+house/@13.0246926,77.569746,17z/data=!3m1!4b1!4m9!4m8!1m1!4e1!1m5!1m1!1s0x3bae17db9ce985b9:0xc21a2bb90740ff4d!2m2!1d77.5704759!2d13.0272127?hl=en>

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- ❖ **Main Guest House (MGH):**

[https://www.google.com/maps/place/13%C2%B001'17.2%22N+77%C2%B034'06.0%22E/@13.0214452,77.5657651,17z/data=!3m1!4b1!4m4!3m3!8m2!3d13.02144!4d77.56834?entry=ttu&g\\_ep=EgoyMDI0MTAyOS4wIKXMDSoASAFQAw%3D%3D](https://www.google.com/maps/place/13%C2%B001'17.2%22N+77%C2%B034'06.0%22E/@13.0214452,77.5657651,17z/data=!3m1!4b1!4m4!3m3!8m2!3d13.02144!4d77.56834?entry=ttu&g_ep=EgoyMDI0MTAyOS4wIKXMDSoASAFQAw%3D%3D)

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❖ **JNC Guest House:**

[https://www.google.com/maps/place/Indian+Institute+Of+Science+Jnc+Guest+House,+Mathikere,+Bengaluru,+Karnataka+560012/@13.0201763,77.5653778,21z/data=!4m6!3m5!1s0x3bae17d71a0e78f7:0xee7499d9a29521c3!8m2!3d13.0202426!4d77.5657481!16s%2Fg%2F11c14796kx?authuser=0&entry=ttu&g\\_ep=EgoyMDI0MTAyOS4wIKXMDSOASAFQAw%3D%3D](https://www.google.com/maps/place/Indian+Institute+Of+Science+Jnc+Guest+House,+Mathikere,+Bengaluru,+Karnataka+560012/@13.0201763,77.5653778,21z/data=!4m6!3m5!1s0x3bae17d71a0e78f7:0xee7499d9a29521c3!8m2!3d13.0202426!4d77.5657481!16s%2Fg%2F11c14796kx?authuser=0&entry=ttu&g_ep=EgoyMDI0MTAyOS4wIKXMDSOASAFQAw%3D%3D)

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❖ **Gokulam Grand Hotel:**

[https://www.google.com/maps/place/Gokulam+Grand+Hotel+%26+Spa/@13.0419696,77.5520584,17z/data=!3m1!4b1!4m9!3m8!1s0x3bae3d5a48506bf5:0x56d985c4fdd0b1d5!5m2!4m1!1i2!8m2!3d13.0419644!4d77.5546333!16s%2Fg%2F1tdbjfgg?authuser=0&entry=ttu&g\\_ep=EgoyMDI0MTAyOS4wIKXMDSOASAFQAw%3D%3D](https://www.google.com/maps/place/Gokulam+Grand+Hotel+%26+Spa/@13.0419696,77.5520584,17z/data=!3m1!4b1!4m9!3m8!1s0x3bae3d5a48506bf5:0x56d985c4fdd0b1d5!5m2!4m1!1i2!8m2!3d13.0419644!4d77.5546333!16s%2Fg%2F1tdbjfgg?authuser=0&entry=ttu&g_ep=EgoyMDI0MTAyOS4wIKXMDSOASAFQAw%3D%3D)

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❖ **Clarion Bangalore Hotel:**

[https://www.google.com/maps/place/Clarion+Bangalore/@13.1089616,77.5577628,17z/data=!3m1!4b1!4m9!3m8!1s0x3bae23f3ce96b937:0x11f8e94ad4216bf!5m2!4m1!1i2!8m2!3d13.1089564!4d77.5603377!16s%2Fg%2F11ns05wj3c?authuser=0&entry=ttu&g\\_ep=EgoyMDI0MTAyOS4wIKXMDSOASAFQAw%3D%3D](https://www.google.com/maps/place/Clarion+Bangalore/@13.1089616,77.5577628,17z/data=!3m1!4b1!4m9!3m8!1s0x3bae23f3ce96b937:0x11f8e94ad4216bf!5m2!4m1!1i2!8m2!3d13.1089564!4d77.5603377!16s%2Fg%2F11ns05wj3c?authuser=0&entry=ttu&g_ep=EgoyMDI0MTAyOS4wIKXMDSOASAFQAw%3D%3D)

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❖ **Hotel Tetrads:**

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SCAN ME



❖ **Hotel Galaxy Suites:**

[https://www.google.com/maps/place/Treebo+Galaxy+Suites+Mathikere/@13.0278386,77.5592379,17z/data=!3m1!4b1!4m10!3m9!1s0x3bae3d3a2ea49ac3:0x9fc89621d894fed!5m3!1s2024-11-04!4m1!1i2!8m2!3d13.0278334!4d77.5618128!16s%2Fg%2F11h92p4r15?entry=ttu&g\\_ep=EgoyMDI0MTAyOS4wIKXMDSOASAFQAw%3D%3D](https://www.google.com/maps/place/Treebo+Galaxy+Suites+Mathikere/@13.0278386,77.5592379,17z/data=!3m1!4b1!4m10!3m9!1s0x3bae3d3a2ea49ac3:0x9fc89621d894fed!5m3!1s2024-11-04!4m1!1i2!8m2!3d13.0278334!4d77.5618128!16s%2Fg%2F11h92p4r15?entry=ttu&g_ep=EgoyMDI0MTAyOS4wIKXMDSOASAFQAw%3D%3D)

SCAN ME



Organized by Team M2S

## Guidelines for Lectures / Poster Presentations

### Guidelines for Plenary Lectures:

All speakers are requested to give their presentation file to the Organizing Team at least half a day before their scheduled presentation. Files in format **.ppt, .pptx and pdf will be accepted in 16 x 9 format.**

Speakers will have 35 minutes for the presentation and 5 minutes for discussions and questions.

### Instructions for Keynote Lecture:

All speakers are requested to give their presentation file to the Organizing Team at least half a day before their scheduled presentation. **Files in format .ppt, .pptx and pdf will be accepted in 16 x 9 format.**

Speakers will have 25 minutes for the presentation, followed by 5 minutes for discussions and questions.

### Instructions for Invited Lectures:

All speakers are requested to give their presentation file to the Organizing Team at least half a day before their scheduled presentation. **Files in format .ppt, .pptx and pdf will be accepted in 16 x 9 format.**

Speakers will have 15 minutes for the presentation, followed by 5 minutes for discussions and questions.

### Instructions for Emerging Researchers' Lectures:

All speakers are requested to give their presentation file to the Organizing Team at least half a day before their scheduled presentation. **Files in format .ppt, .pptx and pdf will be accepted in 16 x 9 format.**

Speakers will have 10 minutes for the presentation, no discussions and questions.

### Instructions for Poster Presentations:

Poster presenters are requested to put their posters on the **morning of 7th November 2024** according to their poster numbers provided near **C-Block Ground floor, Chemical Sciences Division.**

**05.11.2024 (Tuesday)**

Registration: 5<sup>th</sup> November: 8:00 AM-8:30 AM (Chemical Sciences Building Ground Floor)

Inauguration: 8:30 AM - 8:50 AM (AVR Auditorium, CSB 2<sup>nd</sup> floor)

<b>Session 1</b> 8:50 – 9:30	<b>Herre Van Der Zant (AVR)</b> <b>Session Chair: Vadapalli Chandrasekhar</b>		
<b>Session 2</b>	<b>Parallel Session</b>		
<b>Session Chair:</b>	<b>AVR</b> Vadapalli Chandrasekhar	<b>RBM</b> Richard Layfield	
9:30-10:00	Kevin Bernot	Bhavtosh Bansal	
10:00-10:30	Gopalan Rajaraman	Sébastien Pillet	
10:30-11:00	David Brook	Manoranjan Kumar	
11:00-11:20	<b>Tea/Coffee Break</b>		
<b>Session 3</b>	<b>Parallel Session</b>		
<b>Session Chair:</b>	<b>AVR</b> Kevin Bernot	<b>RBM</b> Awadhesh Narayan	
11:20-11:30	<b>ERL: Debopam Sarkar</b>	<b>ERL: Valerio Briganti</b>	
11:30-11:40	<b>ERL: Suraj Halder</b>	<b>ERL: Rishukumar Panday</b>	
11:40-12:00	Srini Kaveri	Prasanta Ghosh	
12:00-12:30	Cyrille Train	Chinmoy Das	
12:30-13:00	David Aguilà	Silvia Gómez-Coca	
13:00-13:50	<b>Lunch Break</b>		
<b>Session 4</b> 13:50-14:30	<b>Masahiro Yamashita (AVR)</b> <b>Session Chair: Dawid Pinkowiz</b>		
<b>Session 5</b>	<b>Parallel Session</b>		
<b>Session Chair:</b>	<b>AVR</b> Dawid Pinkowiz	<b>RBM</b> Pierre Dechambenoit	<b>AG04</b> David Aguilà
14:30-15:00	Jürgen Schnack	Viswanathan Baskar	Itziar Oyarzabal
15:00-15:30	Kanishka Biswas	Saurabh K. Singh	Malcolm Halcrow
15:30-16:00	Mauro Perfetti	Subhadeep Datta	Grace Morgan
16:00-16:30	Anukul Jana	Hiroko Tokoro	Alessia Portieri (ELDICO)
16:30-16:50	<b>Tea/Coffee Break</b>		
<b>Session 6</b>	<b>Parallel Session</b>		
<b>Session Chair:</b>	<b>AVR</b> P. S. Mukherjee	<b>RBM</b> Cyrille Train	<b>AG04</b> Bhagwati Prasad
16:50-17:10	Alex Melville (Cryogenics)	Deepak Asthana	Horiba
17:10-17:40	David A Leigh (Virtual)	Yoshihiro Sekine	17:10-17:30 Guillem Aromi
17:40-18:10	Kasper Pedersen (Virtual)	Atindra N. Pal	17:30-18:00 Ramamoorthy Ramesh
18:10-18:40	Steve Liddle (Virtual)	Kartik V. Raman	18:00-18:30 Henry La Pierre
18:40-19:20	<b>Rigaku International Prize (AVR)</b> Sanjit Konar		
20:00-22:00	<b>Dinner</b>		

<b>Color Code:</b>	<b>AVR Auditorium</b>	<b>RBM Lecture Hall</b>	<b>AG – 04 (Virtual Mode)</b>
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**Organized by Team M2S**

06.11.2024 (Wednesday)			
Session 1 8:50 – 9:30	Vadapalli Chandrasekhar (AVR) Session Chair: Narcis Avarvari		
Session 2	Parallel Session		
Session Chair:	AVR (Miguel Julve Memorial Session) Narcis Avarvari	RBM Satish Patil	AG04 Sheetal Jain
9:30-10:00	Talal Mallah	Sankar P. Rath	Sally Brooker
10:00-10:30	Rodrigue Lescouëzec	Ravindra Venkatramani	Nicholas F. Chilton
10:30-11:00	Marius Andruh	R. Boomi Shankar	
11:00-11:20	Tea/Coffee Break		
Session 3	Parallel Session		
Session Chair:	AVR Shinya Hayami	RBM Anshu Pandey	
11:20-11:30	ERL: Siddhartha De	ERL: Kehkasha Siddiqui	
11:30-11:40	ERL: S. M. Hossain	ERL: Vijay Parmar	
11:40-12:00	Muralidharan Shanmugam	11:40 – 11:50 (ERL) Arpan Mondal	
		11:50 – 12:00 (ERL) Deepanshu Chauhan	
12:00-12:30	Eric Collet	Somobrata Acharya	
12:30-13:00	Satish Patil	Rémi Maurice	
13.00-13.50	Lunch Break		
Session 4 13:50-14:30	Osamu Sato (AVR) Session Chair: Herre Van Der Zant		
Session 5	Parallel Session		
Session Chair:	AVR Herre Van Der Zant	RBM Alessandro Lungi	
14:30-15:00	Lapo Bogani	Shouvik Chatterjee	
15:00-15:30	Matthew J. Cliffe	Indra Dasgupta	
15:30-16:00	Robert Podgajny	Mahesh Sundararajan	
16:00-16:30	Swadhin Mandal	Nathalie Guihéry	
16:30-16:50	Tea/Coffee Break		
Session 6	Parallel Session		
Session Chair:	AVR Rodrigue Lescouëzec	RBM Mathieu Gonidec	AG04 Pradip K Chakraborty
16:50-17:10	Tharamani C. N	Abhishek Banerjee	17:00 – 17:30 Martin Lemaire
17:10-17:40	Narcis Avarvari	Kartik C. Mondal	17:30-18:00 Michael Shatruk
17:40-18:10	Athanasios K Boudalis	Phani K. Peddibhotla	18:00- 18:30 Robert Baker
18:10-18:40	Shinya Hayami	Hélène Bolvin	
18:45-19:45	Cultural Programme (AVR)		
20:00-22:00	Conference Dinner (JVH)		

Color Code:	AVR Auditorium	RBM Lecture Hall	AG – 04 (Virtual Mode)
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**Important Notice!**

The Conference Photograph will be taken on **6th November 2024** before lunch break in front of IISc Main Building



Organized by Team M2S



07.11.2024 (Thursday)		
Session 1 8:50 – 9:30	Arindam Ghosh (AVR) Session Chair: Eric Collet	
Session 2	Parallel Session	
Session Chair:	AVR Eric Collet	RBM Peter Comba
9:30-10:00	Alessandro Lunghi	Masayuki Nihei
10:00-10:30	Vinod C. Prabhakaran	Swapan Pati
10:30-11:00	Dawid Pinkowicz	Ehesan Ali
11:00-11:20	Tea/Coffee Break + Poster	
Session 3	Parallel Session	
Session Chair:	AVR Talal Mallah	RBM Osamu Sato
11:20-11:40	Yanling Li	Kuduva R Vignesh
11:40-12:00	Naitik Panjwani	Sandeep K. Gupta
12:00-12:30	Daniel Talham	Peter Comba
12:30-13:00	Hitoshi Miyasaka	Tomohiro Takayama
13:00-13:50	Lunch Break+ Poster	
Session 4 13:50-14:30	Mario Ruben (AVR) Session Chair: Marius Andruh	
Session 5	Parallel Session	
Session Chair:	AVR Marius Andruh	RBM Soumen Ghosh
14:30-15:00	Aaron Mailman	Fernando Luis
15:00-15:30	Pierre Dechambenoit	Pramod Bhatt
15:30-16:00	Eliseo Ruiz	Pradip K. Chakraborty
16:00-16:30	Matthew P. Shores	Masanori Wakizaka
16:30-16:50	Tea/Coffee Break+ Poster	
Session 6	Parallel Session	
Session Chair:	AVR Matthew J. Cliffe	RBM Daniel Talham
16:50-17:00	ERL: Arup Sarkar	ERL: Abinash Swain
17:00-17:10	ERL: Krishna Kaushik	ERL: Swapnil Shukla
17:10-17:40	Lorenzo Sorace	Satyaprasad P. Senanayak
18:00-19:00	Poster + Light Refreshments	
20:00-22:00	Dinner	

Color Code:	AVR Auditorium	RBM Lecture Hall	AG – 04 (Virtual Mode)
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### Important Notice!



*Poster presenters are requested to put their posters on the morning of 7th November 2024 according to their poster numbers provided near C-Block Ground floor, Chemical Sciences Division.*



Organized by Team M2S

<b>08.11.2024 (Friday)</b>		
<b>Session 1</b> 8:50 – 9:30	<b>Mitsuhiko Maesato (AVR)</b> <b>Session Chair: Fabrice Pointillart</b>	
<b>Session 2</b>	<b>Parallel Session</b>	
<b>Session Chair:</b>	<b>AVR</b> Fabrice Pointillart	<b>RBM</b> Maheswaran Shanmugam
9:30-10:00	Michael L. Baker	Amit Kumar
10:00-10:30	Debamalya Banerjee	Nayanmoni Gogoi
10:30-11:00	Magdalena Fitta	Mathieu Gonidec
11:00-11:20	<b>Tea/Coffee Break</b>	
<b>Session 3</b>	<b>Parallel Session</b>	
<b>Session Chair:</b>	<b>AVR</b> Veerabhadrarao Kaliginedi	<b>RBM</b> Matthew P. Shores
11:20-11:40	Ramanathan Mahendiran	Suranjan Shil
11:40-12:00	Sreetosh Goswami	Vamsee Voora
12:00-12:30	Fabrice Pointillart	Indranil Das
12:30-13:00	Petr Neugebauer	Arun K. Bar
13:00-13:50	<b>Lunch Break</b>	
<b>Session 4</b> 13:50-14:30	<b>Richard Layfield (AVR)</b> <b>Session Chair: Jürgen Schnack</b>	
<b>Session 5</b>	<b>Parallel Session</b>	
<b>Session Chair:</b>	<b>AVR</b> Jürgen Schnack	<b>RBM</b> Gopalan Rajaraman
14:30-15:00	Sergey A. Varganov	Darshan G Joshi
15:00-15:30	Maheswaran Shanmugam	Arun K. Manna
15:30-16:00	Sabyashachi Mishra	Kalobaran Maiti
16:00-16:30	José J. Baldoví	Federico Totti
16:30-16:50	<b>Tea/Coffee Break</b>	
16:50-19:20	<b>Prize Distribution + Closing Ceremony + Remarks</b>	
20:00-22:00	<b>Dinner</b>	

<b>Color Code:</b>	<b>AVR Auditorium</b>	<b>RBM Lecture Hall</b>	<b>AG – 04 (Virtual Mode)</b>
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**Organized by Team M2S**

## Programme Details

Tuesday, 5<sup>th</sup> November 2024

08:00 – 08:30: Registration (Chemical Sciences Division, A-Block, Ground Floor)  
08:30 – 08:50: Inauguration (AVR Auditorium)

### Session – 1:

08:50 – 09:30      **Session Chair**      AVR      Vadapalli Chandrasekhar

08:50 – 09:30	Herre Van Der Zant	Spin switching in single-molecule junctions
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### Session – 2:

09:30 – 11:00      **Session Chair**      AVR      Vadapalli Chandrasekhar  
RBM      Richard Layfield

09:30 – 10:00	Kevin Bernot	Optical and magnetic properties of lanthanide-based supramolecular nanotubes of SCM
	Bhavtosh Bansal	Solid state phase transitions with hysteresis: Mean field universality and beyond
10:00 – 10:30	Gopalan Rajaraman	Electric Field and AI/ML Tools in Advancing Molecular Modelling of Nano Magnets
	Sébastien Pillet	Advanced X-e-N crystallography for molecular switchable and magnetic materials
10:30 – 11:00	David Brook	Electronically Labile Molecules Based on Verdazyl Radicals
	Manoranjan Kumar	Exotic quantum phases in a frustrated spin-1/2 model on a kagome strip chain

11:00 – 11:20	Tea/Coffee Break	
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### Session – 3:

11:20 – 13:00      **Session Chair**      AVR      Kevin Bernot  
RBM      Awadhesh Narayan

11:20 – 11:30 ERL	Debopam Sarkar	Stimuli Responsive Molecular Bistability in discrete Metallosupramolecular Architectures
	Valerio Briganti	Predicting Spin-Phonon Relaxation with Machine Learning
11:30 – 11:40 ERL	Suraj Halder	Spin Decoherence Mechanisms and Mitigation Techniques in Defect-Based Quantum Sensors and Applications
	Rishukumar Panday	Tailoring Ferroelectric Properties in Conformationally Switchable Er(III)-Isothiocyanates Using Organic Cation Modulation
11:40 – 12:00	Srini Kaveri	Funding Opportunities for Research Collaboration in EU, France and CNRS: Tools and mechanisms
	Prasanta Ghosh	Phenoxy Radicals: Proton Coupled Oxidation of Phenol and Diverse Reactivities of Anti-ferromagnetically Coupled and Free Phenoxy radicals
12:00 – 12:30	Cyrille Train	Associating chirality and magnetism in molecule-based systems towards Magneto-chiral and multiferroicity
	Chinmoy Das	Coordination Network-based Glasses: A new frontier of emerging materials
12:30 – 13:00	David Aguilà	Design of H-bonded supramolecular Fe(II) switchable magnetic materials
	Silvia Gómez-Coca	Insights into Single Molecule Magnets, from Blocking temperature to improving spin relaxation by encapsulation

13:00 – 13:50	Lunch Break	
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Organized by Team M2S

**Session – 4:**

13:50 – 14:30

**Session Chair**

AVR

David Pinkowiz

13:50 – 14:30	Masahiro Yamashita	Molecular Spin Qubits toward Quantum Computer and High-Density Memory Devices Based on Molecular Magnets
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**Session – 5:**

14:30 – 16:30

**Session Chair**

AVR

David Pinkowiz

RBM

Pierre Dechambenoit

AG – 04

David Aguilà

14:30 – 15:00	Jürgen Schnack	Exact and approximate theory methods for quantum spin systems
	Viswanathan Baskar	Phosphinates for assembling molecular squares behaving as SMM/SMTs and Organometallic-Inorganic Hybrid Material acting as an Electrocatalyst
	Itziar Oyarzabal	Gd(III)-based complexes as molecular spin qubits
15:00 – 15:30	Kanishka Biswas	Emphasis: Local off-centering of atoms with warming
	Saurabh K. Singh	Molecular Modelling of Ln(III) based Single-Ion Magnets and their Encapsulation in MOFs and Nanotubes
	Malcolm Halcrow	New Insights into the Structural Chemistry of Doped Spin-Crossover Materials
15:30 – 16:00	Mauro Perfetti	Magnetic anisotropy: study, control and exploitation
	Subhadeep Datta	Detection of Magnetism in 2D via Dielectric Measurement
	Grace Morgan	Spin State Ordering and Domain Wall Dynamics in Magnetoelectric Spin Crossover Materials
16:00 – 16:30	Anukul Jana	Redox Mediated Synthesis of Main-Group Based Open-Shell Compounds
	Hiroko Tokoro	Study of Magnetic Domains in Magnetization Reversal on FeCr-hexacyanide magnetic film
	Alessia Portieri (ELDICO)	Electron Diffraction – An Innovative and Advantageous Tool for Structure Determination of Nanocrystalline Materials

**16:30 – 16:50**

**Tea/Coffee Break**

**Session – 6:**

16:50 – 19:20

**Session Chair**

AVR

P. S. Mukherjee

RBM

Cyrille Train

AG – 04

Bhagwati Prasad

16:50 – 17:10	Alex Melville (Cryogenics)	TBA
	Deepak Asthana	Triplet-Triplet Annihilation-based Photochemical Photon Upconversion of Low Intensity Light
	Horiba	TBA
17:10 – 17:40	David A Leigh (Virtual)	Giving Chemistry Direction
	Yoshihiro Sekine	Assembling Prussian Blue Analogs Using Hydrogen Bond-Donating Unit toward Complete Phase Transition
17:10 – 17:30	Guillem Aromi	TBA
17:40 – 18:10	Kasper Pedersen (Virtual)	Molecular Mosaics Losing Their Innocence
	Atindra N. Pal	Electron Transport Through Perfect 1D Atomic/Molecular Chains
17:30 – 18:00	Ramamoorthy Ramesh	Coupling Magnetism To Electricity In Multiferroic Heterostructures
18:10 – 18:40	Steve Liddle (Virtual)	Recent Advances in Actinide-Actinide Bonding: Trithorium Clusters
	Kartik V. Raman	Robust topological Hall effect in ultra-thin Cr <sub>2</sub> Te <sub>3</sub> films by Vanadyl phthalocyanine coupling
18:00 – 18:30	Henry La Pierre	Static and dynamic magnetic properties of tetravalent lanthanide ions



18:40 – 19:20	Rigaku International Prize: Sanjit Konar	Spin-State Switching in Dynamic Molecules and Chiral Cages
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20:00 – 22:00	Dinner	
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**International Conference on  
MODERN TRENDS IN MOLECULAR MAGNETISM- IV  
AND  
SPINS IN MOLECULAR SYSTEMS: EXPERIMENT,  
THEORY AND APPLICATIONS-III**

**Rigaku International Prize**  
Awarded to  
**Prof. Sanjit Konar**  
Indian Institute of Education and Research, Bhopal



5<sup>th</sup> to 8<sup>th</sup> November 2024  
Website: <https://mtmm-sims2024.in/>




**International Conference on  
MODERN TRENDS IN MOLECULAR MAGNETISM- IV  
AND  
SPINS IN MOLECULAR SYSTEMS: EXPERIMENT,  
THEORY AND APPLICATIONS-III**

**Miguel Julve Olcina Memorial Lecture Series**  
6<sup>th</sup> November 2024,  
AVR Auditorium, 9:30 AM – 11:00 AM




Session Chair:  
Narcis Avarvari



Speaker:  
Talal Mallah



Speaker:  
Rodrigue Lescouëzec



Speaker:  
Marius Andruh

5<sup>th</sup> to 8<sup>th</sup> November 2024  
Website: <https://mtmm-sims2024.in/>




**Organized by Team M2S**

Wednesday, 6<sup>th</sup> November 2024

Session – 1:

08:50 – 09:30      Session Chair      AVR      Narcis Avarvari

08:50 – 09:30	Vadapalli Chandrasekhar	Synthetic Strategies for the Assembly of Mononuclear, Dinuclear and Tetranuclear Lanthanide Complexes
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Session – 2:

09:30 – 11:00      Session Chair      AVR      Narcis Avarvari  
RBM      Satish Patil  
AG – 04      Sheetal Jain

09:30 – 10:00	Talal Mallah	Magnetic molecules based on transition metal ions as spin quantum bits
	Sankar P. Rath	Metal vs. Ligand Oxidation: Electronic Communication through Bridge and Spin Coupling
	Sally Brooker	TBA
10:00 – 10:30	Rodrigue Lescouëzec	Molecular Switches based on Metal-Metal Electron Transfer
	Ravindra Venkatramani	Electronic Molecular Breadboards
	Nicholas F. Chilton	Accurate and Efficient Spin-Phonon Coupling and Spin Dynamics Calculations for Molecular Solids
10:30 – 11:00	Marius Andruh	Combined $2p/3d/4f$ chemistry: new synthetic routes towards magnetic materials
	R. Boomi Shankar	Molecular Ferroelectrics Derived from Switchable Metal-Ligand Coordination

11:00 – 11:20      Tea/Coffee Break

Session – 3:

11:20 – 13:00      Session Chair      AVR      Shinya Hayami  
RBM      Anshu Pandey

11:20 – 11:30 ERL	Siddhartha De	Electron delocalisation and multicenter bonding in metallolebased dimeric lanthanide complexes
	Kehkasha Siddiqui	Magnetic Behaviour of Cationic, Mononuclear, Air-stable Cobalt(II) Phosphoric Triamide Complexes
11:30 – 11:40 ERL	S. M. Hossain	Modulation of Spin Crossover Behaviour via Photosalient Structural Transformation
	Vijay Parmar	Multi-technique study of the magnetic anisotropy in Co(II) Single Molecule Magnets
11:40 – 12:00	Muralidharan Shanmugam	Mechanism of Co-C Bond Cleavage in B12-Dependent Photoreceptor and the Intermediates probed by Crystallography, UV-Vis and cw-EPR/annealing Methods
11:40 – 11:50 ERL	Arpan Mondal	Masked Divalent Reactivity of Heterobimetallic Lanthanide Isocarbonyl Complexes
11:50 – 12:00 ERL	Deepanshu Chauhan	Room Temperature Giant Magnetolectric Coupling for Magnetic Energy Harvesting in Single Phase $\{Co^{III}_3Dy^{III}\}$ Molecular Nanogenerator
12:00 – 12:30	Eric Collet	From Ultrafast Photoinduced Small Polarons to Cooperative and Macroscopic Charge-Transfer Phase Transition
	Somobrata Acharya	Unveiling Solid State Luminescence from Ultra-thin Noncovalent Two-dimensional Molecular Crystals Fabricated at Air-Water Interface
12:30 – 13:00	Satish Patil	Spin Evolution in Molecular Structures
	Rémi Maurice	Meticulous extraction of the multispin Hamiltonian in dicobalt(II) complexes out of ab initio calculations

**13:00 – 13:50** Conference Photograph @ IISc Main Building & Lunch Break

**Session – 4:**

13:50 – 14:30 **Session Chair** AVR Herre Van Der Zant

13:50 – 14:30	Osamu Sato	Electric polarization control via electron transfer
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**Session – 5:**

14:30-16:30 **Session Chair** AVR Herre Van Der Zant  
RBM Alessandro Lungi

14:30 – 15:00	Lapo Bogani	Quantum Control of Molecular Carbon
	Shouvik Chatterjee	Controlling Hall response in epitaxial Mn <sub>3</sub> Sn thin films
15:00 – 15:30	Matthew J. Cliffe	Modular metal-organic materials towards unconventional function
	Indra Dasgupta	Tailoring Spin Textures in Non-centrosymmetric Systems
15:30 – 16:00	Robert Podgajny	Spins in multicomponent cyanidometallate-based systems: selective spin state switching and optical properties
	Mahesh Sundararajan	Electronic Structures of High-Valent Metal Complexes with Diverse Spin States
16:00 – 16:30	Swadhin Mandal	From Spin Materials to Electron Transfer Catalysis
	Nathalie Guihéry	How to create giant anisotropic interactions in poly-nuclear magnetic systems and impact of the electric field on anisotropic interactions: New insights from theory

**16:30 – 16:50** Tea/Coffee Break

**Session – 6:**

16:50 – 18:40 **Session Chair** AVR Rodrigue Lescouëzec  
RBM Mathieu Gonidec  
AG – 04 Pradip K Chakraborty

16:50 – 17:10	Tharamani C. N	Designing greener energy conversion system for a sustainable future
	Abhishek Banerjee	Investigations into the Electrochemical Energy Storage Properties of Diphosphonate derivatives of Oxo-vanadates: Experiment and Theory
17:00 – 17:30	Martin T. Lemaire	Exploring single-component spin-crossover conductors using redox-active ligands
17:10 – 17:40	Narcis Avarvari	Chirality Induced Spin Selectivity (CISS) effect with helicene and tetrathiafulvalene derivatives
	Kartik C. Mondal	Electronic Structures of Stable Metal-Radical Complexes
17:30 – 18:00	Michael Shatruk	TBA
17:40 – 18:10	Athanassios K Boudalis	Spin triangles: from magnetoelectric couplings to spin-electric transitions
	Phani K. Peddibhotla	High sensitivity magnetometry with quantum defects in diamond
18:00 – 18:30	Robert Baker	Probing Spin Polarized Electron Dynamics in Yttrium Iron Garnet Using Circularly Polarized XUV Light
18:10 – 18:40	Shinya Hayami	Spin Crossover System with Multifunction
	Hélène Bolvin	Probing the magnetic properties of actinide complexes by paramagnetic NMR

**18:45 – 19:45** Cultural Program (AVR Auditorium)

**20:00 – 22:00** Conference Dinner (JVH)



**Important Notice!**

*The Conference Photograph will be taken on 6th November 2024 before lunch break in front of IISc Main Building*



**Organized by Team M2S**



**Thursday, 7<sup>th</sup> November 2024**

**Session – 1:**

08:50 – 09:30      **Session Chair**      AVR      Eric Collet

08:50 – 09:30	Arindam Ghosh	Engineering interfaces in metals for strong charge-lattice-spin coupling
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**Session – 2:**

09:30 – 11:00      **Session Chair**      AVR      Eric Collet  
RBM      Peter Comba

09:30 – 10:00	Alessandro Lunghi	Computational Design of Magnetic Molecules
	Masayuki Nihei	Molecular Prussian Blue Analogues: From Bulk to Molecules and Low-dimensional Aggregates
10:00 – 10:30	Vinod C. Prabhakaran	Nailing the Holy Grail of Methane Partial Oxidation
	Swapan Pati	Computational Modeling of Competing Magnetic Phases, Quantum Spin Liquid Candidates and Molecular Magnets
10:30 – 11:00	Dawid Pinkowicz	Reversible Photochemistry And Magnetism Of Cyanide-bridged Molecular Solids
	Ehesan Ali	Exchange Interactions Induced Magnetization Relaxation in Single Molecule Magnets

**11:00 – 11:20      Tea/Coffee Break & Poster Session**

**Session – 3:**

11:20 – 13:00      **Session Chair**      AVR      Talal Mallah  
RBM      Osamu Sato

11:20 – 11:40	Yanling Li	Cyanide-bridged Fe <sub>2</sub> Co <sub>2</sub> tetranuclear complexes-Contribution of pressure study to the comprehension of magnetic switching
	Kuduva R Vignesh	Role of 3d/4d-4f magnetic exchange interactions and diamagnetic 3d ions on the Ln(III) magnetic dynamics in heterometallic {3d/4d-4f} SMMs
11:40 – 12:00	Naitik Panjwani	Optically addressable spin states in fully organic diradicals probed by spin resonance techniques
	Sandeep K. Gupta	Maximizing the Magnetic Anisotropy in Four-Coordinate Cobalt(II) Single-Ion Magnets
12:00-12:30	Daniel Talham	Interface and Matrix Effects on Spin Transition Solids
	Peter Comba	Modeling Spin for Applications of Metal Complexes
12:30-13:00	Hitoshi Miyasaka	Magnetic Sponges for Switching
	Tomohiro Takayama	Development of candidate materials for Kitaev spin liquid

**13:00-13:50      Lunch Break & Poster Session**

**Session – 4:**

13:50-14:30      **Session Chair**      AVR      Marius Andruh

13:50 – 14:30	Mario Ruben	Quantum Computing with Molecules
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**Session – 5:**

14:30-16:30	<b>Session Chair</b>	AVR	Marius Andruh
		RBM	Soumen Ghosh

14:30 – 15:00	Aaron Mailman	Achieving Thermal Hysteresis in Neutral and Ionic Main Group Radicals
	Fernando Luis	Wiring up Molecular Spin Qudits with Superconducting Circuits
15:00 – 15:30	Pierre Dechambenoit	How and why promoting large spin delocalization in molecule-based magnets?
	Pramod Bhatt	Prussian Blue Analogues Molecular Magnets: Pigments to Power
15:30 – 16:00	Eliseo Ruiz	From Single-Molecule to 2D Layers: Magnetism and Transport
	Pradip K. Chakraborty	Unraveling Structure-property Interplay in Fe(II) and Co(II) Spin-crossover Coordination Networks: A Fascinating Diversity
16:00 – 16:30	Matthew P. Shores	Elucidating and controlling intermolecular interactions for magnetic switching
	Masanori Wakizaka	Quantum magnetism of Co(II) and Cu(II) centers in metalorganic frameworks and in molecular-chains

<b>16:30 – 16:50</b>	<b>Tea/Coffee Break &amp; Poster Session</b>
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**Session – 6:**

16:50 – 18:20	<b>Session Chair</b>	AVR	Matthew J. Cliffe
		RBM	Daniel Talham

16:50 – 17:00 ERL	Arup Sarkar	Deciphering the Origin of Double Exchange and Magnetic Exchange in a [Fe <sub>3</sub> ] Cluster using Density Matrix Renormalization Group (DMRG) Approach
	Abinash Swain	Qubits Within Transition Metal Helicates: Encased Molecular Structures
17:00 – 17:10 ERL	Krishna Kaushik	Multifunctionality in cyanobridged coordination networks
	Swapnil Shukla	Molecular Clusters to Ladders: Designing unprecedented low dimensional Fe-Cu based heterobimetallic cyanometallates
17:10 – 17:40	Lorenzo Sorace	Exchange coupling and spin parity effects on the magnetization dynamics of Lanthanide-based complexes: an NMR and $\mu$ SR investigation
	Satyaprasad P. Senanayak	Switching in Unconventional Semiconductors

<b>18:00 – 19:00</b>	<b>Poster Session &amp; Light Refreshments</b>
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<b>20:00 – 22:00</b>	<b>Dinner</b>
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Friday, 8<sup>th</sup> November 2024

Session – 1:

08:50 – 09:30      Session Chair      AVR      Fabrice Pointillart

08:50 – 09:30	Mitsuhiko Maesato	Quantum Spin Liquids in Triangular-Lattice Organic Mott Insulators
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Session – 2:

09:30 – 11:00      Session Chair      AVR      Fabrice Pointillart  
RBM      Maheswaran Shanmugam

09:30 – 10:00	Michael L. Baker	Quantifying single-ion magnet dynamics with X-ray spectroscopies
	Amit Kumar	Understanding of magnetization reversal and its correlations with other physical properties
10:00 – 10:30	Debamalya Banerjee	Exploring Spin Multiplicity in MoS <sub>2</sub>
	Nayanmoni Gogoi	Engineering Water Processable Multifunctional Molecular Magnetic Materials
10:30 – 11:00	Magdalena Fitta	Stimuli-responsive electrospun composites based on molecular magnets and organic polymers
	Mathieu Gonidec	The challenges and rewards of preparing self-assembled monolayers of functional coordination compounds on metallic substrates

11:00 – 11:20      Tea/Coffee Break

Session – 3:

11:20 – 13:00      Session Chair      AVR      Veerabhadrarao Kaliginedi  
RBM      Matthew P. Shores

11:20 – 11:40	Ramanathan Mahendiran	Giant magnetostriction in perovskite oxides
	Suranjan Shil	Effect of orbital manipulation to tune the magnetic interaction in organic diradicals
11:40 – 12:00	Sreetosh Goswami	Molecular Neuromorphic Building Blocks for Artificial Intelligence
	Vamsee Voora	Polarization Induced Quantum Confinement of Negative Charge Carriers by Organic Nanoporous Frameworks
12:00 – 12:30	Fabrice Pointillart	Circularly Polarized Luminescence in Single-Molecule Magnets
	Indranil Das	Synergy of Electronic Band Topology and Non-Trivial Magnetism
12:30 – 13:00	Petr Neugebauer	Rapid scan ESR: A Versatile Tool for the Spin Relaxation Studies at (sub)THz Frequencies
	Arun K. Bar	CO <sub>2</sub> gas as a resource for deriving lanthanide(III) magnetic motifs: tailoring SMM behavior via post-synthetic inner coordination modification

13:00 – 13:50      Lunch Break

Session – 4:

13:50-14:30      Session Chair      AVR      Jürgen Schnack

13:50 – 14:30	Richard Layfield	Organometallic Approaches to Lanthanide SMMs
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Session – 5:



Organized by Team M2S



**MODERN TRENDS IN MOLECULAR MAGNETISM – IV**  
**&**  
**SPINS IN MOLECULAR SYSTEMS:**  
**EXPERIMENT, THEORY AND APPLICATIONS – III**



14:30 – 16:30

**Session Chair**

AVR  
RBM

Jürgen Schnack  
Gopalan Rajaraman

14:30 – 15:00	Sergey A. Varganov	Nonadiabatic molecular dynamics with the crystal field Hamiltonian to study spin dynamics in lanthanide complexes
	Darshan G Joshi	Topological excitations in quantum magnets
15:00 – 15:30	Maheswaran Shanmugam	TBA
	Arun K. Manna	Computational Design of Metal-Free Functional Organic Molecules for Efficient Triplet Photosensitization
15:30 – 16:00	Sabyashachi Mishra	Quantum Chemistry on a Quantum Device: Algorithm and Application
	Kalobaran Maiti	Anomalies and Kink in topological Kondo lattice systems
16:00 – 16:30	José J. Baldoví	Engineering 2D magnetism in van der Waals materials using first principles
	Federico Totti	Elective Affinities: when Molecular Magnets Meet the Surface

<b>16:30 – 16:50</b>	<b>Tea/Coffee Break</b>
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<b>16:50-19:20</b>	<b>Prize Distribution , Closing Ceremony , Remarks (AVR Auditorium)</b>
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<b>20:00 – 22:00</b>	<b>Dinner</b>
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**Organized by Team M2S**

## Plenary Lectures

Lecture No.	Speaker Name	Title of the Lecture
PL01	Herre Van Der Zant	Spin switching in single-molecule junctions
PL02	Masahiro Yamashita	Molecular Spin Qubits toward Quantum Computer and High-Density Memory Devices Based on Molecular Magnets
PL03	Osamu Sato	Electric polarization control via electron transfer
PL04	Vadapalli Chandrasekhar	Synthetic Strategies for the Assembly of Mononuclear, Dinuclear and Tetranuclear Lanthanide Complexes
PL05	Arindam Ghosh	Engineering interfaces in metals for strong charge-lattice-spin coupling
PL06	Mario Ruben	Quantum Computing with Molecules
PL07	Mitsuhiro Maesato	Quantum Spin Liquids in Triangular-Lattice Organic Mott Insulators
PL08	Richard Layfield	Organometallic Approaches to Lanthanide SMMs



## Keynote Lectures

Lecture No.	Speaker Name	Title of the Lecture
KL01	Kevin Bernot	Optical and magnetic properties of lanthanide-based supramolecular nanotubes of SCM
KL02	Bhavtosh Bansal	Solid state phase transitions with hysteresis: Mean field universality and beyond
KL03	Gopalan Rajaraman	Electric Field and AI/ML Tools in Advancing Molecular Modelling of Nano Magnets
KL04	Sébastien Pillet	Advanced X-e-N crystallography for molecular switchable and magnetic materials
KL05	David Brook	Electronically Labile Molecules Based on Verdazyl Radicals
KL06	Manoranjan Kumar	Exotic quantum phases in a frustrated spin-1/2 model on a kagome strip chain
KL07	Cyrille Train	Associating chirality and magnetism in molecule-based systems towards Magneto-chiral and multiferroicity
KL08	Chinmoy Das	Coordination Network-based Glasses: A new frontier of emerging materials
KL09	David Aguilà	Design of H-bonded supramolecular Fe(II) switchable magnetic materials
KL10	Silvia Gómez-Coca	Insights into Single Molecule Magnets, from Blocking temperature to improving spin relaxation by encapsulation
KL11	Jürgen Schnack	Exact and approximate theory methods for quantum spin systems
KL12	Viswanathan Baskar	Phosphinates for assembling molecular squares behaving as SMM/SMTs and Organometallic-Inorganic Hybrid Material acting as an Electrocatalyst
KL13	Itziar Oyarzabal	Gd(III)-based complexes as molecular spin qubits
KL14	Kanishka Biswas	Emphasis: Local off-centering of atoms with warming
KL15	Saurabh K. Singh	Molecular Modelling of Ln(III) based Single-Ion Magnets and their Encapsulation in MOFs and Nanotubes
KL16	Malcolm Halcrow	New Insights into the Structural Chemistry of Doped Spin-Crossover Materials

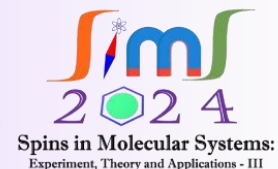
KL17	<b>Mauro Perfetti</b>	Magnetic anisotropy: study, control and exploitation
KL18	<b>Subhadeep Datta</b>	Detection of Magnetism in 2D via Dielectric Measurement
KL19	<b>Grace Morgan</b>	Spin State Ordering and Domain Wall Dynamics in Magnetoelectric Spin Crossover Materials
KL20	<b>Anukul Jana</b>	Redox Mediated Synthesis of Main-Group Based Open-Shell Compounds
KL21	<b>Hiroko Tokoro</b>	Study of Magnetic Domains in Magnetization Reversal on FeCr-hexacyanide magnetic film
KL22	<b>Alessia Portieri (ELDICO)</b>	Electron Diffraction – An Innovative and Advantageous Tool for Structure Determination of Nanocrystalline Materials
KL23	<b>David A. Leigh</b>	Giving Chemistry Direction
KL24	<b>Yoshihiro Sekine</b>	Assembling Prussian Blue Analogs Using Hydrogen Bond-Donating Unit toward Complete Phase Transition
KL25	<b>Kasper Pedersen</b>	Molecular Mosaics Losing Their Innocence
KL26	<b>Atindra N Pal</b>	Electron Transport Through Perfect 1D Atomic/Molecular Chains
KL27	<b>Ramamoorthy Ramesh</b>	Coupling Magnetism To Electricity In Multiferroic Heterostructures
KL28	<b>Steve Liddle</b>	Recent Advances in Actinide-Actinide Bonding: Trithorium Clusters
KL29	<b>Kartik V. Raman</b>	Robust topological Hall effect in ultra-thin Cr <sub>2</sub> Te <sub>3</sub> films by Vanadyl phthalocyanine coupling
KL30	<b>Henry La Pierre</b>	Static and dynamic magnetic properties of tetravalent lanthanide ions
KL31	<b>Talal Mallah</b>	Magnetic molecules based on transition metal ions as spin quantum bits
KL32	<b>Sankar P. Rath</b>	Metal vs. Ligand Oxidation: Electronic Communication through Bridge and Spin Coupling
KL33	<b>Sally Brooker</b>	TBA
KL34	<b>Rodrigue Lescouëzec</b>	Molecular Switches based on Metal-Metal Electron Transfer
KL35	<b>Ravindra Venkatramani</b>	Electronic Molecular Breadboards

KL36	<b>Marius Andruh</b>	Combined 2p/3d/4f chemistry: new synthetic routes towards magnetic materials
KL37	<b>R. Boomi Sankar</b>	Molecular Ferroelectrics Derived from Switchable Metal-Ligand Coordination
KL38	<b>Nicholas F. Chilton</b>	Accurate and Efficient Spin-Phonon Coupling and Spin Dynamics Calculations for Molecular Solids
KL39	<b>Eric Collet</b>	From Ultrafast Photoinduced Small Polarons to Cooperative and Macroscopic Charge-Transfer Phase Transition
KL40	<b>Somobrata Acharya</b>	Unveiling Solid State Luminescence from Ultra-thin Noncovalent Two-dimensional Molecular Crystals Fabricated at Air-Water Interface
KL41	<b>Satish Patil</b>	Spin Evolution in Molecular Structures
KL42	<b>Remi Maurice</b>	Meticulous extraction of the multispin Hamiltonian in dicobalt(II) complexes out of ab initio calculations
KL43	<b>Lapo Bogani</b>	Quantum Control of Molecular Carbon
KL44	<b>Shouvik Chatterjee</b>	Controlling Hall response in epitaxial Mn <sub>3</sub> Sn thin films
KL45	<b>Matthew J. Cliffe</b>	Modular metal-organic materials towards unconventional function
KL46	<b>Indra Dasgupta</b>	Tailoring Spin Textures in Non-centrosymmetric Systems
KL47	<b>Robert Podgajny</b>	Spins in multicomponent cyanidometallate-based systems: selective spin state switching and optical properties
KL48	<b>Mahesh Sundararajan</b>	Electronic Structures of High-Valent Metal Complexes with Diverse Spin States
KL49	<b>Swadhin K. Mandal</b>	From Spin Materials to Electron Transfer Catalysis
KL50	<b>Nathalie Guihéry</b>	How to create giant anisotropic interactions in poly-nuclear magnetic systems and impact of the electric field on anisotropic interactions: New insights from theory
KL51	<b>Martin T Lamire</b>	Exploring single-component spin-crossover conductors using redox-active ligands
KL52	<b>Narcis Avarvari</b>	Chirality Induced Spin Selectivity (CISS) effect with helicene and tetrathiafulvalene derivatives
KL53	<b>Kartik C. Mondal</b>	Electronic Structures of Stable Metal-Radical Complexes
KL54	<b>Michael Shatruk</b>	TBA

KL55	<b>Athanassios K Boudalis</b>	Spin triangles: from magnetoelectric couplings to spin-electric transitions
KL56	<b>Phani K. Peddibhotla</b>	High sensitivity magnetometry with quantum defects in diamond
KL57	<b>Robert Baker</b>	Probing Spin Polarized Electron Dynamics in Yttrium Iron Garnet Using Circularly Polarized XUV Light
KL58	<b>Shinya Hayami</b>	Spin Crossover System with Multifunction
KL59	<b>Hélène Bolvin</b>	Probing the magnetic properties of actinide complexes by paramagnetic NMR
KL60	<b>Alessandro Lungi</b>	Computational Design of Magnetic Molecules
KL61	<b>Masayuki Nihei</b>	Molecular Prussian Blue Analogues: From Bulk to Molecules and Low-dimensional Aggregates
KL62	<b>Vinod C. Prabhakaran</b>	Nailing the Holy Grail of Methane Partial Oxidation
KL63	<b>Swapan Pati</b>	Computational Modeling of Competing Magnetic Phases, Quantum Spin Liquid Candidates and Molecular Magnets
KL64	<b>Dawid Pinkowicz</b>	Reversible Photochemistry And Magnetism Of Cyanide-bridged Molecular Solids
KL65	<b>Ehesan Ali</b>	Exchange Interactions Induced Magnetization Relaxation in Single Molecule Magnets
KL66	<b>Daniel Talham</b>	Interface and Matrix Effects on Spin Transition Solids
KL67	<b>Peter Comba</b>	Modeling Spin for Applications of Metal Complexes
KL68	<b>Hitoshi Miyasaka</b>	Magnetic Sponges for Switching
KL69	<b>Tomohiro Takayama</b>	Development of candidate materials for Kitaev spin liquid
KL70	<b>Aaron Mailman</b>	Achieving Thermal Hysteresis in Neutral and Ionic Main Group Radicals
KL71	<b>Fernando Luis</b>	Wiring up Molecular Spin Qudits with Superconducting Circuits
KL72	<b>Pierre Dechambenoit</b>	How and why promoting large spin delocalization in molecule-based magnets?
KL73	<b>Pramod Bhatt</b>	Prussian Blue Analogues Molecular Magnets: Pigments to Power



**MODERN TRENDS IN MOLECULAR MAGNETISM – IV**  
**&**  
**SPINS IN MOLECULAR SYSTEMS:**  
**EXPERIMENT, THEORY AND APPLICATIONS – III**



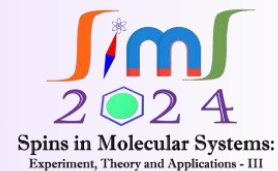
KL74	<b>Eliseo Ruiz</b>	From Single-Molecule to 2D Layers: Magnetism and Transport
KL75	<b>Pradip K. Chakraborty</b>	Unraveling Structure-property Interplay in Fe(II) and Co(II) Spin-crossover Coordination Networks: A Fascinating Diversity
KL76	<b>Matthew P. Shores</b>	Elucidating and controlling intermolecular interactions for magnetic switching
KL77	<b>Masanori Wakizaka</b>	Quantum magnetism of Co(II) and Cu(II) centers in metalorganic frameworks and in molecular-chains
KL78	<b>Lorenzo Sorace</b>	Exchange coupling and spin parity effects on the magnetization dynamics of Lanthanide-based complexes: an NMR and mSR investigation
KL79	<b>Satyaprasad P. Senanayak</b>	Switching in Unconventional Semiconductors
KL80	<b>Michael L. Baker</b>	Quantifying single-ion magnet dynamics with X-ray spectroscopies
KL81	<b>Amit Kumar</b>	Understanding of magnetization reversal and its correlations with other physical properties
KL82	<b>Debamalya Banerjee</b>	Exploring Spin Multiplicity in MoS <sub>2</sub>
KL83	<b>Nayanmoni Gogoi</b>	Engineering Water Processable Multifunctional Molecular Magnetic Materials
KL84	<b>Magdalena Fitta</b>	Stimuli-responsive electrospun composites based on molecular magnets and organic polymers
KL85	<b>Mathieu Gonidec</b>	The challenges and rewards of preparing self-assembled monolayers of functional coordination compounds on metallic substrates
KL86	<b>Fabrice Pointillart</b>	Circularly Polarized Luminescence in SingleMolecule Magnets
KL87	<b>Indranil Das</b>	Synergy of Electronic Band Topology and NonTrivial Magnetism
KL88	<b>Petr Neugebauer</b>	Rapid scan ESR: A Versatile Tool for the Spin Relaxation Studies at (sub)THz Frequencies
KL89	<b>Arun K Bar</b>	CO <sub>2</sub> gas as a resource for deriving lanthanide(III) magnetic motifs: tailoring SMM behavior via post-synthetic inner coordination modification
KL90	<b>Sergey A. Varganov</b>	Nonadiabatic molecular dynamics with the crystal field Hamiltonian to study spin dynamics in lanthanide complexes
KL91	<b>Darshan G. Joshi</b>	Topological excitations in quantum magnets
KL92	<b>Maheswaran Shanmugam</b>	TBA



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**MODERN TRENDS IN MOLECULAR MAGNETISM – IV**  
&  
**SPINS IN MOLECULAR SYSTEMS:**  
**EXPERIMENT, THEORY AND APPLICATIONS – III**



KL93	<b>Arun K. Manna</b>	Computational Design of Metal-Free Functional Organic Molecules for Efficient Triplet Photosensitization
KL94	<b>Sabyasachi Mishra</b>	Quantum Chemistry on a Quantum Device: Algorithm and Application
KL95	<b>Kalobaran Maiti</b>	Anomalies and Kink in topological Kondo lattice systems
KL96	<b>José J. Baldoví</b>	Engineering 2D magnetism in van der Waals materials using first principles
KL97	<b>Federico Totti</b>	Elective Affinities: when Molecular Magnets Meet the Surface



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## Invited Lectures

Lecture No.	Speaker Name	Title of the Lecture
IL01	Srini Kaveri	Funding Opportunities for Research Collaboration in EU, France and CNRS: Tools and mechanisms
IL02	Prasanta Ghosh	Phenoxy Radicals: Proton Coupled Oxidation of Phenol and Diverse Reactivities of Anti-ferromagnetically Coupled and Free Phenoxy
IL03	Alex Melville	TBA
IL04	Deepak Asthana	Triplet-Triplet Annihilation-based Photochemical Photon Upconversion of Low Intensity Light
IL05	Horiba	TBA
IL06	Guillem Aromi	TBA
IL07	Muralidharan Shanmugam	Mechanism of Co-C Bond Cleavage in B12-Dependent Photoreceptor and the Intermediates probed by Crystallography, UV-Vis and cwEPR/annealing Methods
IL08	Tharamani C.N	Designing greener energy conversion system for a sustainable future
IL09	Abhishek Banerjee	Investigations into the Electrochemical Energy Storage Properties of Diphosphonate derivatives of Oxo-vanadates: Experiment and Theory
IL10	Yanling Li	Cyanide-bridged Fe <sub>2</sub> Co <sub>2</sub> tetranuclear complexes- Contribution of pressure study to the comprehension of magnetic switching
IL11	Kuduva R Vignesh	Role of 3d/4d-4f magnetic exchange interactions and diamagnetic 3d ions on the Ln(III) magnetic dynamics in heterometallic {3d/4d-4f} SMMs
IL12	Naitik Panjwani	Optically addressable spin states in fully organic diradicals probed by spin resonance techniques
IL13	Sandeep K. Gupta	Maximizing the Magnetic Anisotropy in FourCoordinate Cobalt(II) Single-Ion Magnets
IL14	Ramanathan Mahendiran	Giant magnetostriction in perovskite oxides
IL15	Suranjan Shil	Effect of orbital manipulation to tune the magnetic interaction in organic diradicals
IL16	Sreetosh Goswami	Molecular Neuromorphic Building Blocks for Artificial Intelligence
IL17	Vamsee Voora	Polarization Induced Quantum Confinement of Negative Charge Carriers by Organic Nanoporous Frameworks

## Emerging Researchers' Lectures (ERLs)

Name	Affiliation	Title of the talk / Poster
Dr. Abinash Swain	University of Barcelona, Spain	Qubits Within Transition Metal Helicates: Encased Molecular Structures
Dr. Arpan Mondal	University of Sussex, UK	Masked Divalent Reactivity of Heterobimetallic Lanthanide Isocarbonyl Complexes
Dr. Arup Sarkar	Trinity College Dublin, Ireland	Deciphering the Origin of Double Exchange and Magnetic Exchange in a [Fe <sub>3</sub> ] Cluster using Density Matrix Renormalization Group (DMRG) Approach
Mr. Debopam Sarkar	IISc Bangalore, India	Stimuli Responsive Molecular Bistability in discrete Metallosupramolecular Architectures
Mr. Deepanshu Chauhan	IIT Bombay, India	Room Temperature Giant Magnetoelectric Coupling for Magnetic Energy Harvesting in Single Phase {CoII3DyIII} Molecular Nanogenerator
Ms. Kehkasha Siddiqui	IIT Bombay, India	Magnetic Behaviour of Cationic, Mononuclear, Air-stable Cobalt(II) Phosphoric Triamide Complexes
Ms. Krishna Kaushik	IISc Bangalore, India	Multifunctionality in Cyanobridged Coordination Networks
Mr. Rishukumar Panday	IISER Pune, India	Tailoring Ferroelectric Properties in Conformationally Switchable Er(III)-Isothiocyanates Using Organic Cation Modulation
Dr. Sayed Muktar Hossain	Gurudas College, India	Modulation of Spin Crossover Behaviour via Photosalient Structural Transformation
Dr. Siddhartha De	University of Sussex, UK	Electron delocalisation and multicenter bonding in metallolebased dimeric lanthanide complexes
Mr. Suraj Halder	IISc Bangalore, India	Spin Decoherence Mechanisms and Mitigation Techniques in Defect-Based Quantum Sensors and Applications.
Mr. Swapnil Shukla	IISc Bangalore, India	Molecular Clusters to Ladders: Designing unprecedented low dimensional Fe-Cu based heterobimetallic cyanometallates
Mr. Valerio Briganti	Trinity College Dublin, Ireland	Predicting Spin-Phonon Relaxation with Machine Learning
Dr. Vijay Singh Parmar	Aarhus University, Denmark	Multi-technique study of the magnetic anisotropy in Co(II) Single Molecule Magnets



## Poster Presentations

Poster No.	Name of the Participant	Affiliation	Title of the talk / Poster
P01	Abhirami R. J.	Vellore Institute of Technology, India	Magnetic and Electronic Properties of FeCO and FeC <sub>2</sub> O Molecules: A Computational Study
P02	Abinash Swain (ERL)	University of Barcelona, Spain	Qubits Within Transition Metal Helicates: Encased Molecular Structures
P03	Amit Gharu	IISER Mohali, India	Single-molecule magnetic and Single-molecule toric behavior of 3d-4f complexes
P04	Anuj Kumar Ray	IACS Kolkata, India	Unlocking simple features to predict DFT spin state gaps of 3d metal complexes using Machine Learning
P05	Anup Choudhury	Handique Girls' College, Guwahati, India	Post-synthetic miniaturization of multifunctional chiral cyanido-bridged Mn(II)-Fe(III)/W(V) network
P06	Arindam Gupta	IISER Bhopal, India	Interplay of lattice cooperativity and elastic frustration influencing SCO behaviour in two Fe <sup>II</sup> -[Ag(CN) <sub>2</sub> ] Hofmann CPs with distinct interpenetrated structures
P07	Arpan Mondal (ERL)	University of Sussex, UK	Masked Divalent Reactivity of Heterobimetallic Lanthanide Isocarbonyl Complexes
P08	Bapan Jana	IIT Bombay, India	A Molecular Based Piezoelectric Nanogenerator for Sustainable Energy Harvesting using a ferroelectric Co(II) complex
P09	Bhart Kumar	IISER, Bhopal, India	Image processing affords temperature mapping using a spin crossover based thermochromic sensor
P10	Calvin Samuel P	University of Hyderabad, India	Metal- $\pi$ Interaction: An Unconventional Approach Towards Hybrid Material and its Efficacy in Electrocatalytic Reduction of Nitrate to Ammonia
P11	Ch Mudasar Hussain	JNU Delhi, India	Synthesis and Isolation of Stable Naphthalenediimide-based Radical Cation and Dication
P12	Chandan Panigrahy	IIT Bombay, India	Effect of spin state on Photocatalytic Reactivity of Non Heme Iron(IV)=O Complexes
P13	Chumuiria Debbarma	Manipal University, India	Spin Dynamics and Magnetic Behaviour of Organic Diradicals on Graphene Surface: Insights from computational studies
P14	Daniele Sartini	University of Florence, Italy	TBA
P15	Debopam Sarkar (ERL)	IISc Bangalore, India	Stimuli Responsive Molecular Bistability in discrete Metallosupramolecular Architectures

P16	Deepanshu Chauhan (ERL)	IIT Bombay, India	Room Temperature Giant Magnetolectric Coupling for Magnetic Energy Harvesting in Single Phase $\{Co^{III}_3Dy^{III}\}$ Molecular Nanogenerator
P17	Dipanti Borah	IIT Bombay, India	An Unprecedented Square Planar Fe(III) Complex Exhibiting Spin Crossover Between the Spin-Admixed States
P18	Esha Gera	IISER Mohali, India	An In-Depth Evaluation of Systematic Benchmarking of Reported Systems and Synergistic Experimental and Computational Investigation of Fe-tetraazatricyclo Complexes
P19	Garima Bangar	IIT Bombay, India	Achieving Ambient Stability and Suppressing Spin-Phonon Coupling in Dyprosocenium SIMs via MOF Encapsulation
P20	Himanshu Gupta	University of Pennsylvania, USA	Synthesis and Electronic Structure Studies of an Ytterbium-Pyrazine Square complex
P21	Ibtesham Tarannum	IIT Hyderabad, India	Unravelling Electronic Structure, Bonding, and Magnetic Properties of Dysprosium Complexes
P22	Ihjas Aslam K K	Pondicherry University, India	Rational Design of Ferromagnetic Graphene by Selective Hydrogenation
P23	Imon jyoti Dutta	IISER Mohali, India	In pursuit of 4d/5d-4f Single Molecule Magnets
P24	N. Johnee Britto	IIT Bombay, India	Decoding the Electronic Origins of Outer-Sphere & Inner-Sphere Electron Transfer in High-Valent Non-Heme Metal-oxo Species
P25	K. Vignesh	IIT Bombay, India	TBA
P26	Kehkasha Siddiqui (ERL)	IIT Bombay, India	Magnetic Behaviour of Cationic, Mononuclear, Air-stable Cobalt(II) Phosphoric Triamide Complexes
P27	Krishna Kaushik (ERL)	IISc Bangalore, India	Multifunctionality in cyanobridged coordination networks
P28	Krishna Kumar M S	JNU Delhi, India	Multiple redox-states crystallized by controlled electrocrystallization
P29	Manikandan Marimuthu	National University of Singapore, Singapore	Anomalous Nernst Effect and Giant Magnetostriction in Microwave processed $La_{0.5}Sr_{0.5}CoO_3$
P30	Manjeet Kumar	IIT Bombay, India	Unveiling the Role of Magnetic Exchange in Metal-Superoxo Species for C-H Bond Activation Reactions
P31	Muskan	Manipal University, India	Magnetic Coupling and Spintronics properties of Helical Phenalene Diradicals
P32	Naitik A. Panjwani	Berlin Joint EPR Lab, Fachbereich Physik, Freie Universität, Germany	Optically addressable spin states in fully organic diradicals probed by spin resonance techniques
P33	Naman Kumar Bharti	Homi Bhabha National Institute Mumbai, India	Efficient Water Splitting with a Semiconductor based Supramolecular Catalyst

P34	Neeraj Singh Dhauni	IIT Bombay, India	Deciphering the Origin of Double Exchange and Magnetic Exchange in a [Fe <sub>3</sub> ] Cluster using Density Matrix Renormalization Group (DMRG) Approach
P35	Neha Sharma	IISER Mohali, India	TBA
P36	Niku Ahmed	Tezpur University, India	Self-Assembly of Cyano-Bridged [CoFe] Molecular Dimers: Synthesis and Characterization
P37	Parthajit Chakravarty	Pondicherry University, India	In silico Investigation of Magnetic Properties of Heteroatom-doped Graphene (C7X, X= N, B)
P38	Prajesh Neetu	IISER Pune, India	A Ferroelectric Two-Dimensional Metal-Organic Coordination Polymer Showing Piezoelectric Energy Harvesting Properties
P39	Purva Dua	IIT Bombay, India	Unravelling the Mechanism of CO <sub>2</sub> Activation: Insights into Metal-Metal Cooperativity and Spin-Orbit Coupling with {3d–4f} Catalysts
P40	R Arulkumar	IIT Bombay, India	The Interplay of Spin States, Ligands, and Additives in High Valent Metal–Oxo Mediated C–H Activation: A Computational Study
P41	Rahul Sutradhar	IACS Kolkata, India	Mechanistic investigations of C-H activation by various spin states of [Co <sup>III,IV</sup> <sub>2</sub> (μ-O) <sub>2</sub> ] diamond core complex
P42	Rajanikanta Rana	IIT Bombay, India	A Machine Learning Approach to Decipher the Origin of Magnetic Anisotropy in Three-Coordinate Cobalt Single-Ion Magnets
P43	Rajdeep Paul	IIT Bombay, India	Investigating the Influence of Oriented External Electric Fields on Modulating Spin-Transition Temperatures in Fe(II) SCO Complexes: A Theoretical Perspective
P44	Ranjan Kharel	IISER, Bhopal, India	Solvent Orchestrates Photo-responsive Behavior in cyanide bridged Fe <sub>2</sub> Co Single-Chain Magnet
P45	Rishukumar Panday (ERL)	IISER Pune, India	Tailoring Ferroelectric Properties in Conformationally Switchable Er(III)-Isothiocyanates Using Organic Cation Modulation
P46	Rupesh Kr. Tiwari	IIT Bombay, India	Enhancing Spin-Transport Characteristics, Spin-Filtering Efficiency, and Negative Differential Resistance in Exchange-Coupled Dinuclear Co(II) Complexes for Molecular Spintronics Applications
P47	Sadananda Kumbhakar	IIT Bombay, India	Pyridine backbone di-peptide based metal free organic materials as piezoelectric energy harvesters
P48	Sanjoy Sarkar	Tezpur University, India	Tris-hydrazone ligand based C <sub>3</sub> -Symmetric trinuclear Ln-clusters in the perspective of Single-Molecule Toroids

P49	Satheeshkumar M	IIT Bombay, India	Fine-Tuning the FT-AFT Gap in {CrDy <sub>6</sub> } Complex through Electron Donating and Withdrawing Group Effects: A Combined Experimental and Theoretical Approach
P50	Sayed Muktar Hossain (ERL)	Gurudas College, West Bengal, India	Modulation of Spin Crossover Behaviour via Photosensitive Structural Transformation
P51	Shintaro Akagi	University of Tsukuba, Japan	Metamagnetic properties in two types of Ni-W cyanide assemblies
P52	Shirsha Saha	Pondicherry University, India	Ferromagnetism in Porphyrinic Based 2D Sheets
P53	Shraoshee Shome	IISER Bhopal, India	The effect of conjugation in tuning the SMM and luminescence thermometry of two di-nuclear lanthanide complexes
P54	Shruti Moorthy	IIT Hyderabad, India	Computational Insights into Modulating Magnetic Anisotropy in Mononuclear Single-Molecule Magnets
P55	Siddhartha De (ERL)	University of Sussex, UK	Electron delocalisation and multicenter bonding in metallobased based dimeric lanthanide complexes
P56	Sukanya Bagchi	IISc Bangalore, India	Modulating Magnetic Anisotropy and Luminescence in Lanthanide Complexes and its Application as SMM Transistor
P57	Sunita Sharma	IIT Bombay, India	Role of Coupling Strength, Cooperativity, and Covalency Dictating the C–H Bond Activation Reactivity in Ni <sub>2</sub> E <sub>2</sub> (E = O, S, Se, and Te) Complexes
P58	Suraj Halder (ERL)	IISc Bangalore, India	Spin Decoherence Mechanisms and Mitigation Techniques in Defect-Based Quantum Sensors and Applications
P59	Suresh Swain	IIT Bombay, India	Exploring Spin Transport Characteristics of Mixed-Valence {V <sup>IV</sup> -V <sup>III</sup> } Magnetic Dimer: Probing the Interplay of Magnetic-Exchange and Double-Exchange Effects
P60	Susanta Manna	IISc Bangalore, India	Misfit Layered Nanotubes from La <sub>1-x</sub> Y <sub>x</sub> S-TaS <sub>2</sub> : Influence of Charge Transfer on Superconductivity and Charge Density Waves
P61	Swapnil Shukla (ERL)	IISc Bangalore, India	Molecular Clusters to Ladders: Designing unprecedented low dimensional Fe-Cu based heterobimetallic cyanometallates
P62	Tanu Sharma	IIT Bombay, India	Role of Oxidation State on Anisotropy and the Spin-Phonon Relaxation in Single-Ion Magnets
P63	Tapaswini Sethi	JNU Delhi, India	Temperature induced kinematic effect: Jumping, splitting spinning and running of an organic salt crystal

<b>P64</b>	Thakur Rochak Kumar Rana	IIT Bombay, India	Role of Spin Crossover in Covalent Modification of Amino Acids in Cytochrome P460 Cofactor Maturation
<b>P65</b>	Vaibhav Singh	IISER Tirupati, India	Lanthanide Mediated Utilization of Aerial CO <sub>2</sub> Towards Designing Efficient Single Molecule Magnets
<b>P66</b>	Valerio Briganti (ERL)	Trinity College Dublin, Ireland	Predicting Spin-Phonon Relaxation with Machine Learning
<b>P67</b>	Veeramani Rajendran	IISc Bangalore, India	Unveiling the Local Atomic Structure of Cr-Implanted InGaO <sub>3</sub> Superlattices to Correlate with Infrared Emission Luminescence
<b>P68</b>	Vijay Singh Parmar (ERL)	Aarhus University, Denmark	Multi-technique study of the magnetic anisotropy in Co(II) Single Molecule Magnets
<b>P69</b>	Vijaya Thangaraj	IIT Bombay, India	Quantifying Magnetic Anisotropy of Series of Five-coordinate Co(II) ions: Experimental and Theoretical Insights
<b>P70</b>	Vipanchi	IISER Mohali, India	Exploring the magnetic behavior of {Ln <sub>2</sub> } Single Molecule Magnets with diverse bridging ligands. Synthesis and theoretical Insights
<b>P71</b>	Yugal Kishore Kausalya	Pondicherry University, India	Metal-Free Ferromagnetism in B <sub>12</sub> based 2D sheets: Oxidation Induced by Electronegative Bridges



## Speakers for Day 1 : 5<sup>th</sup> November 2024

- 1) Herre Van Der Zant
- 2) Kevin Bernot
- 3) Bhavtosh Bansal
- 4) Gopalan Rajaraman
- 5) Sébastien Pillet
- 6) David Brook
- 7) Manoranjan Kumar
- 8) Debopam Sarkar (ERL)
- 9) Valerio Briganti (ERL)
- 10) Suraj Halder (ERL)
- 11) Rishukumar Panday (ERL)
- 12) Srini Kaveri
- 13) Prasanta Ghosh
- 14) Cyrille Train
- 15) Chinmoy Das
- 16) David Aguilà
- 17) Silvia Gómez-Coca
- 18) Masahiro Yamashita
- 19) Jürgen Schnack
- 20) Viswanathan Baskar
- 21) Itziar Oyarzabal
- 22) Kanishka Biswas
- 23) Saurabh K. Singh
- 24) Malcolm Halcrow
- 25) Mauro Perfetti
- 26) Subhadeep Datta
- 27) Grace Morgan
- 28) Anukul Jana
- 29) Hiroko Tokoro
- 30) Alessia Portieri (ELDICO)
- 31) Alex Melville (Cryogenics)
- 32) Deepak Asthana
- 33) Horiba
- 34) David A Leigh (Virtual)
- 35) Yoshihiro Sekine
- 36) Guillem Aromi
- 37) Kasper Pedersen (Virtual)
- 38) Atindra N. Pal
- 39) Ramamoorthy Ramesh
- 40) Steve Liddle (Virtual)
- 41) Kartik V. Raman
- 42) Henry La Pierre
- 43) Rigaku International Prize: Sanjit Konar



## Spin switching in single-molecule junctions

Herre S.J. van der Zant

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We have developed several techniques to fabricate single-molecule devices, in which a single molecule bridges the gap between two electrodes. Devices include (gated) mechanical controlled break junctions, junctions made with a self-breaking electromigration technique and room-temperature stable molecular transistors formed by electroburning few-layer graphene. Often a third gate electrode is present [1] that allows the modification of charge transport independently from the source/drain electrodes thereby realizing a transistor in which the electric current through the molecule probes its properties. Using these different techniques, quantum transport phenomena [2] are studied in a wide variety of (magnetic) molecules including mono-radicals, bi- and tri-radicals, single-molecule magnets (SMMs) and spin-crossover compounds.

In this talk I will discuss the magnetic fingerprints present in single-molecule transport while concentrating on junctions containing spin-crossover compounds. I will show how the low- to high-spin transition can be triggered by an electric field when introducing dipole moments on the molecule or by mechanical stretching [3]. Spin-state dependent conductance switching is also studied with graphene electrodes and shown to occur well below the critical temperature for crystals of the same molecules. Calculations suggest that switching at the single-molecule level can be induced by small perturbations to the ligand distance in the molecular junction. In the above mentioned cases, the spin crossover compound contains a Fe ion; we will also discuss recent results on the electric field switching of a Mn spin-crossover compound in a single molecule break junction.

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## Optical and magnetic properties of lanthanide-based supramolecular nanotubes of SCM

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Several years of our work on lanthanide-based magnetic molecules<sup>1</sup> and in particular Ln-based single-chain magnets (SCM) will be reviewed. We will illustrate how SCM behavior can be observed on lanthanide–radical chains with original topologies such as chiral molecular nanotubes<sup>2</sup> and their derivatives derivatives.<sup>3</sup> Then, we will illustrate how metallogels can be formed from these objects while preserving their morphologic and magnetic properties.<sup>4</sup> Moreover, the creation of thick films as well as submonolayer deposits of supramolecular nanotubes on surface will be evidenced.<sup>5</sup> Last, recent findings on enantiopure gels of nanotubes of SCM and their optical properties will be commented.



**Figure 1** Supramolecular nanotubes of SCM as solution, gels and surface deposits

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# Solid state phase transitions with hysteresis: Mean field universality and beyond

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Many thermally-driven abrupt structural transitions in solid-state systems are observed to be always hysteretic [1]. Based on the understanding gained primarily from the study of the phase transitions in the transition metal oxides ( $V_2O_3$ ,  $VO_2$ , and  $NdNiO_3$ ) and halide perovskites ( $MAPbX_3$ ), I will argue that these must be distinguished from the usual first-order transitions on the account of long-range interactions.

We have observed slowing down of the order parameter fluctuations accompanied by their enhanced variance ('critical opalescence'), and dynamic scaling around the phase transition in these systems [2]. These features which are associated with second-order transitions suggest that the abrupt transition is controlled by a critical-like singularity. The singularities are identified with the spinodal points and vindicate Van der Waals' original mean-field theory for the phase transitions, without Maxwell's correction.

I will also describe observations beyond the mean-field scenario, emphasizing the athermal and disorder landscape aspects of these transitions. The ability of these materials to hierarchically encode a large number of metastable configurations via their thermal history and their possible use as memory materials will be highlighted.

## References and Notes

1. Examples include spin-crossover materials, transition metal oxides underdoing the metal-insulator transition, magnetic intermetallic alloys, manganites, charge density wave compounds, metal hydrides, ammonium chloride, quartz, transitions to incommensurate structures in dielectrics, and halide perovskites.
2. Tapas Bar, *et al.*, *Phys. Rev. Lett.* 121, 045701 (2018); S. Kundu, *et al.*, *Phys. Rev. Lett.* 124, 095703 (2020) ; S. Kundu, *et al.*, *Phys. Rev. E* 108, 024101 (2023).



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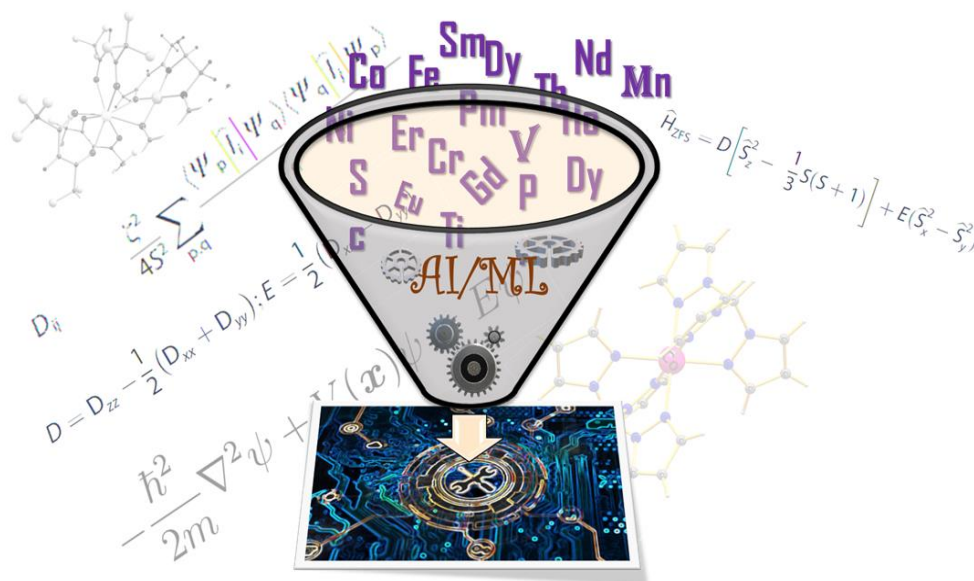
# Electric Field and AI/ML Tools in Advancing Molecular Modelling of Nano Magnets

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Molecular magnetism is one of the vastly growing research fields with an aim to design molecules and materials with tunable magnetic and electronic properties.<sup>Error! Reference source not found.</sup> Their synthesis, characterization and implementation as devices create a lively crossroad among chemistry, physics and material science: a multidisciplinary research field. These molecules have widespread potential applications ranging from magnetic storage devices, spintronics, and Q-bits in quantum computing to magnetic coolants.<sup>Error! Reference source not found.</sup> Single-molecule magnets (SMMs) are the molecules which show slow relaxation of magnetization below the critical temperature and exhibit a hysteresis loop similar to classical magnets. SMMs offer key advantages over classical magnets due to their lightweight, solubility and multifunctional behaviour. Theoretical tools are indispensable in this arena<sup>2</sup> for understanding the observed magnetic properties. The strength of these methods is not only limited to rationalization but also the prediction of novel molecules which can exhibit superior magnetic properties. In this presentation, I will research the effort undertaken by our group towards achieving this goal.<sup>2, 3</sup>



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## Advanced X-e-N crystallography for molecular switchable and magnetic materials

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The precise understanding of the mechanisms at the origin of the physical properties in molecular crystals, nanocrystals or even nanocomposites, strongly rely on our ability to describe the structural architecture on a multi-scale basis. For that purpose, scattering techniques using X-rays, electrons or neutrons have their own respective advantages. In that presentation, advanced methods allowing to retrieve the structure in equilibrium and out of equilibrium states of molecular magnetic and switchable materials will be reviewed. Recent quantum crystallography approaches will be introduced as well.



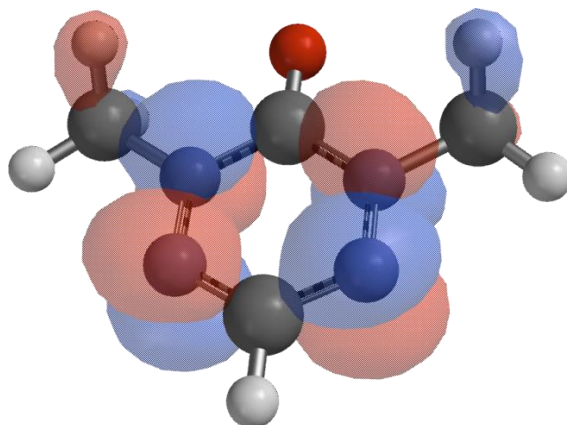
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## Electronically Labile Molecules Based on Verdazyl Radicals

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Electronically labile molecules are those in which the electronic structure is very sensitive to the molecular environment. Such molecules can typically switch between states that exhibit different electronic distributions and spin multiplicity. Changes in the environment can result in dramatic changes in magnetic properties and molecular geometry which may have both sensing and information storage applications. Because of their versatile structure, reversible redox activity, and potential to act as ligands to metal ions, we have found that verdazyls are key components to building electronically labile systems. Examples include spin crossover influenced by electron or proton transfer and valence tautomerism influenced by temperature and crystal packing. These systems present not only remarkable physical properties, but also significant theoretical challenges in describing their electronic structure. We will discuss examples that include both purely organic systems and metal coordination compounds, including some more recent results with cobalt-verdazyl and copper-verdazyl systems.



**Figure 1** Structure and SOMO of a prototypical verdazyl free radical.



## Exotic quantum phases in a frustrated spin-1/2 model on a kagomestrip chain

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We investigate the quantum phases of a frustrated antiferromagnetic Heisenberg spin-1/2 model Hamiltonian on a Kagome strip chain (KSC), a one-dimensional analogue of the kagome lattice, and construct the quantum phase diagram in their two-dimensional exchange parameter space. The isolated unit cell of this lattice comprises five spin-1/2 particles, giving rise to three types of magnetic states: spin- $3/2$  state, spin- $1/2$  state with orbital degree of freedom, and spin- $1/2$  state with dimerized base spins at every unit cell, depending on the exchange ratio within the unit cell. We explore the ground state properties of this model in the interacting spin-1/2 unit cell using exact diagonalization and density matrix renormalization group methods, identifying five distinct quantum phases. Two types of dimerized ground states emerge due to doubly degenerate ground states breaking inversion symmetry. Notably, the first phase (Phase III) exhibits gapless spin excitation, while the second phase (Phase IV) has a finite but small spin gap due to translation symmetry breaking. The remaining phases exhibit gapless spectra with antiferromagnetic quasi-long-range order in the central spins. In Phase I, the unit cell spin is  $3/2$ , and in Phase II, base spins of neighboring unit cells form singlet dimers. In the phase V phase, base spins form strong singlet dimers, and the central spin-1/2 creates an isotropic effective spin-1/2 chain. Additionally, we develop an effective model incorporating both spin-1/2 and orbital degrees of freedom, resembling the Kugel-Khomskii model with highly anisotropic orbital degrees of freedom



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## Stimuli Responsive Molecular Bistability in discrete Metallosupramolecular Architectures

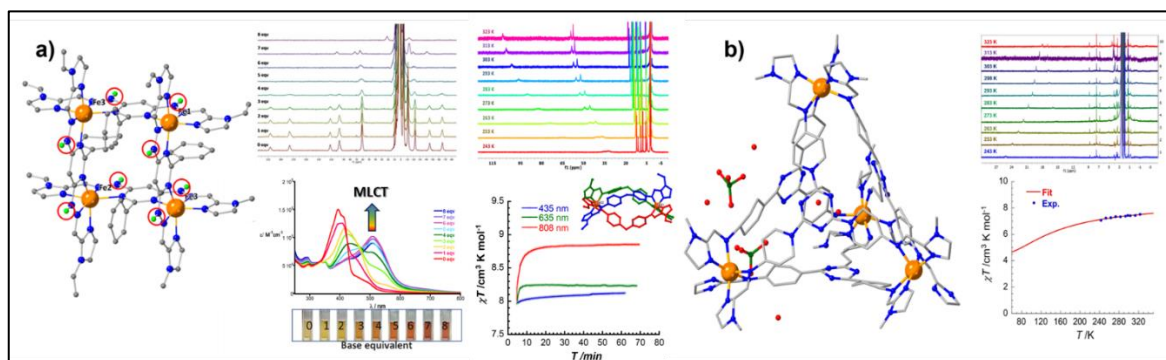
Debopam Sarkar,<sup>a</sup> Sounak Ghosh,<sup>a</sup> Prof. Abhishake Mondal<sup>\*a</sup>

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Potential application of molecular magnetic materials in future electronic devices depends on the “molecular bistability” between two easily accessible electronic spin states of the system i.e., high spin (HS) and low spin (LS). The bistability of these materials occurs under influence of external stimuli such as light, temperature, pressure etc<sup>1</sup>. Constructing elegant and intricate molecular systems following nature mimicking self-assembly process gives us a unique wealth of metallosupramolecular architectures that is employed to design and synthesize switchable molecular magnetic materials stemming from the strong communication and co-operativity between the metal centres inside supramolecular framework.<sup>2</sup> These discrete complexes are not only useful for switching application but also have other uses such as sensing and separation, catalysis and biotechnology.<sup>2</sup> Herein, I represent different metallosupramolecular architectures comprising Fe(II) based tetrahedral cages, [2X2] grids and dinuclear helicates with interesting switching characteristics both in solid and solution state under application of external stimuli.



**Figure 1 (a)** Structure of Fe(II) [2X2] grid and helicate showing switching of Spin State in solution with change in pH and temperature, respectively; **(b)** Structure of Fe(II) tetrahedral cage and variable temperature Evans <sup>1</sup>H-NMR

**Acknowledgement:** We thank the Solid State and Structural Chemistry Unit, Indian Institute of Science, Scheme for Transformational and Advanced Research in Sciences (STARS), Ministry of Education, and Prime Minister’s Research Fellowship, MoE, Government of India.

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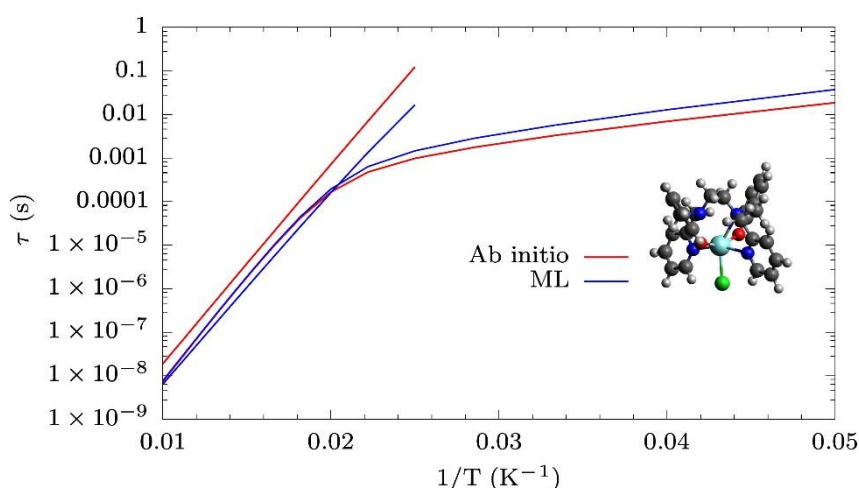
## Predicting Spin-Phonon Relaxation with Machine Learning

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The interaction of the spin of single molecule magnets (SMMs) with phonons is the main cause of decoherence and relaxation towards equilibrium at room temperature, hindering the usage of these systems as platforms for quantum technologies. A full ab-initio approach based on the combination of the theory of open quantum systems with methods of quantum chemistry permits to reach high precision in spin dynamics simulations [1], but it requires conspicuous computational resources. The main focus of this contribution is on machine learning and its application to overcome this bottleneck at multiple stages, from the geometrical optimization to the generation of reliable molecular dynamics (MD) trajectories and prediction of tensorial properties. For this purpose, I will present a linear model for the description of force fields along with an active learning strategy to efficiently select configurations to include in the training set [2]. Results will be presented for the prediction of phonon frequencies for Co and Dy based SMMs, their profiles of spin-relaxation time versus temperature (see Fig.1) and for the efficient prediction of correlation functions of spin Hamiltonian tensors onto MD trajectories several ns long.



**Fig. 1.** Relaxation profiles obtained with full ab initio method and with phonons predicted with machine learning force fields for a Dy compound.

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# Spin Decoherence Mechanisms and Mitigation Techniques in Defect-Based Quantum Sensors and Applications.

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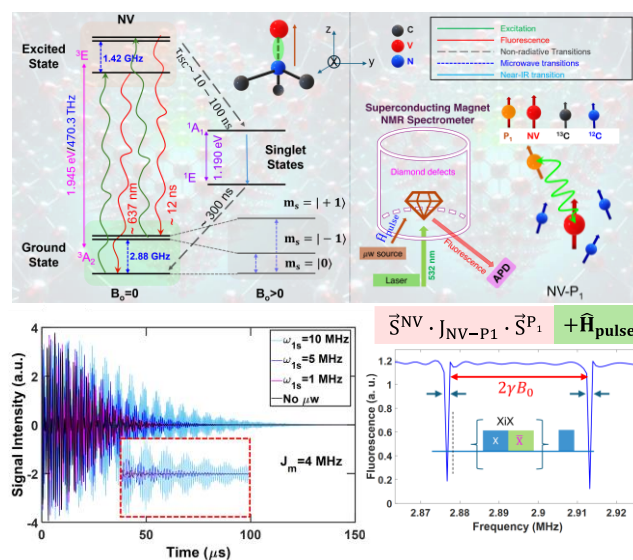
Corresponding author e-mail: [skj@iisc.ac.in](mailto:skj@iisc.ac.in)

Quantum sensing (QS) and quantum information science (QIS) are rapidly evolving fields that leverage quantum systems to enhance sensing, computing, and communication. Key systems include nitrogen-vacancy (NV) centers in diamond, hexagonal boron nitride (hBN), and silicon carbide (SiC), valued for their controllable spins and optical addressability. NV centers are particularly attractive due to their long coherence times, which can be improved by optimizing material designs to minimize hyperfine interactions through NMR-active isotopes. To achieve precise control over coherence times in defect-based systems, advanced techniques such as microwave ( $\mu\text{W}$ ) or radiofrequency (RF) pulse sequences are essential for reducing anisotropic interactions. We investigated the root causes of decoherence, focusing on spin-spin interactions like NV-nuclear spin hyperfine coupling and fluctuations in NV-NV or NV- $P_1$  dipolar coupling<sup>1,2</sup>. While traditional dynamic decoupling methods like Hahn-echo<sup>3</sup> primarily target hyperfine coupling, recent studies show that  $P_1$  center interactions significantly affect decoherence pathways. Fluctuations in dipolar coupling can shorten coherence time to under  $40 \mu\text{s}$  for an NV- $P_1$  cluster, but continuous microwave irradiation or repetitive two  $\pi$  pulses (XiX) can extend it beyond  $120 \mu\text{s}$ . We utilize MATLAB simulations to assess the effects of these couplings on decoherence, aiming to optimize decoupling pulse applications to enhance coherence times and sensitivity in ODMR.

**Keywords:**  $P_1$  center, dipolar-coupling, decoupling sequences or XiX, ODMR<sup>4</sup>.

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**Figure 1.** Top left: the energy diagram of the NV center. The top right: the dipolar coupling between NV- $P_1$ . The bottom: the numerical result of the application of the decoupling pulse and effect in ODMR spectrum.



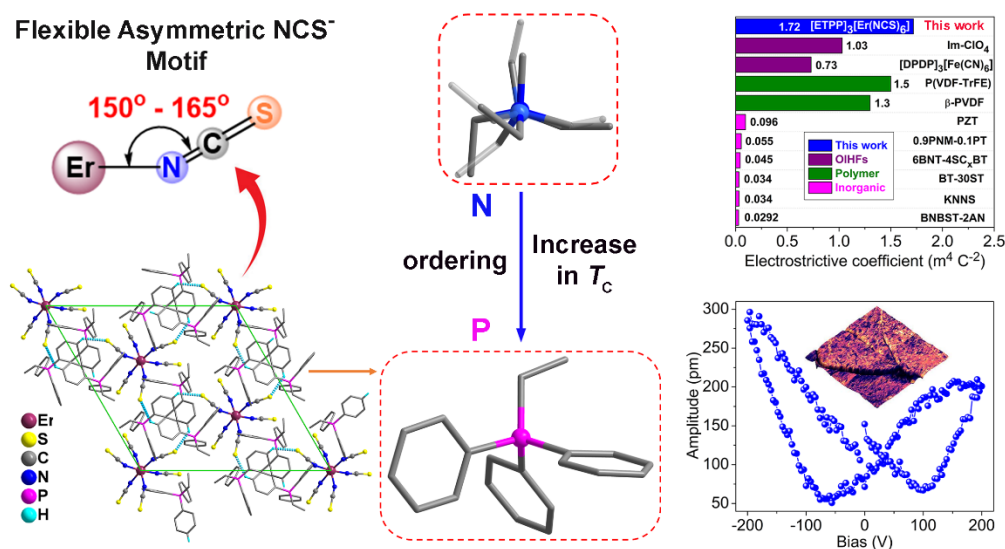
# Tailoring Ferroelectric Properties in Conformationally Switchable Er(III)-Isothiocyanates Using Organic Cation Modulation

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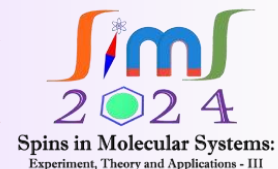
Hybrid molecular ferroelectrics, due to their facile synthesis and robust physical properties, have emerged as a new class of functional materials. Such systems require flexible parts that can lock into two different positions and thereby switch the polarity of the crystal in a reversing electric field. Isothiocyanate ligands display this kind of behavior in their usual non-linear coordination. In homoleptic complexes of lanthanide ions, they often have varying coordination numbers, which can be controlled by the size of the counterions. Using triethyl methyl ammonium (TEMA) cations yields the salt [TEMA]<sub>4</sub>[Er(NCS)<sub>7</sub>] that shows a phase transition denoted by the Aizu notation *mmmFmm2* at 203 K. In contrast, the bulkier phosphonium cation ethyltriphenyl phosphonium (ETPP) yielded the high-*T<sub>c</sub>* (or effectively *T<sub>c</sub>*-free) ferroelectric [ETPP]<sub>3</sub>[Er(NCS)<sub>6</sub>]. The polarization vs. electric field (*P-E*) loop measurements on a single crystal gave a saturation polarization (*P<sub>s</sub>*) of 4.33 μC cm<sup>-2</sup>, while dielectric measurements revealed the absence of a paraelectric phase (*T<sub>c</sub>*) close to the melting point (483 K). It also exhibits the piezoelectric charge coefficient (*d*<sub>33</sub>) of 22.7 pC N<sup>-1</sup>, the highest amongst the phosphonium-based organic and hybrid materials, and electrostrictive coefficient (*Q*<sub>33</sub>) of 1.72 m<sup>4</sup> C<sup>-2</sup>, far exceeding those of earlier reported lead-free hybrid materials and organic polymers. Ferroelectric domain analysis and polarization switching from piezoresponse force microscopy (PFM) corroborate the multiaxial polarization nature of [ETPP]<sub>3</sub>[Er(NCS)<sub>6</sub>]. Finally, thermoplastic polyurethane composite devices of [ETPP]<sub>3</sub>[Er(NCS)<sub>6</sub>] were investigated for mechanical energy harvesting applications.



**Figure 1.** Designing strategy of molecular ferroelectrics and its high piezoresponse behavior from conformationally switchable Er(III)-NCS motif.

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## Funding Opportunities for Research Collaboration in EU, France and CNRS: Tools and mechanisms

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In a global village-like scenario, the societal challenges including health issues, demographic change, climate change, need for clean and efficient energy, smart and integrated transport, food security, and the bio-based economy, are all global. Addressing these new challenges warrants answers that are also ought to be global and more importantly, there is a need for urgent solutions. An efficient international cooperation assisting a link between scientific research and industrial leadership is an absolute necessity to address these tasks.

The **European Union** has made significant efforts in this direction through several of its international collaborative research programs. As a case study, we will consider the initiatives that the **French government** presents to support and enhance the Indo-French scientific collaborations.

Further, we present an overview of CEFIPRA, the Indo-French Centre, and the international collaborative programs of “Centre National de la Recherche Scientifique” commonly known as **CNRS**. CNRS has put in place several mechanisms to establish scientific cooperation between international scientific community and the CNRS labs. These mechanisms include International Emerging Actions, International Research Networks, International Research Programs among others.

In this presentation, we intend to provide a synopsis of the mechanisms that facilitate interaction between India and EU with an emphasis on France and on CNRS.



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# Phenoxy Radicals: Proton Coupled Oxidation of Phenol and Diverse Reactivities of Anti-ferromagnetically Coupled and Free Phenoxy

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In this presentation, the effect of the intermolecular H-bonding to the concerted proton coupled electron transfer (CPET) reactions of phenols affording H-bonded phenoxy radicals are analyzed.<sup>1</sup> In this project, salts containing intermolecular iminium-phenolato H-bonds, [(Zn)Ar-O<sup>-</sup>---(-<sup>+</sup>HN)=CH-Ar] that undergo CPET reactions in air producing [Ar-O---HO-Ar]<sup>•</sup> were successfully isolated. The phenoxy radicals are presented in two forms, [(Zn)Ar-O<sup>•</sup>---HO-Ar (zinc phenoxy) ↔ (Zn)Ar-OH---<sup>•</sup>O-Ar (free phenoxy)]. The phenoxy radical form was justified by X-ray bond parameters, EPR signals, phenol to phenoxy inter-valence charge transfer (IVCT) transitions and spin density distribution. The potential shift due to CPET reactions facilitated by H-bonding was estimated by cyclic voltammetry.

Further, it is disclosed that the reactivities of the anti-ferromagnetically coupled and uncoupled phenoxy radicals coordinated to metal ions are diverse.<sup>2</sup> It has been observed that the coupled [Ru<sup>III</sup>-phenoxy] leads to an intramolecular redox reaction oxidizing one of the ligands and undergoes dimerization producing a binuclear ruthenium (III) complex with a strong Ru-Ru bond, while the uncoupled [Ru<sup>II</sup>-phenoxy] promotes an intermolecular redox reaction facilitating C-C radical coupling and H-abstraction reactions. The coupling reaction affords a 4,4'-biphenylsemiquinone anion radical complex, while the H-abstraction reaction reverts the [Ru<sup>II</sup>-phenoxy] to a [Ru<sup>II</sup>-Phenol] complex. Also, the coupled and uncoupled *o*-iminobenzosemiquinone anion radical forms coordinated to ruthenium (III/II) were successfully isolated and authenticated, however no such reactions of these *o*-iminobenzosemiquinone anion radicals were observed.

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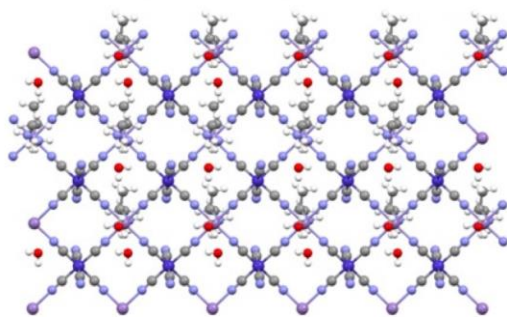
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## Associating chirality and magnetism in molecule-based systems towards Magneto-chiral and multiferroicity

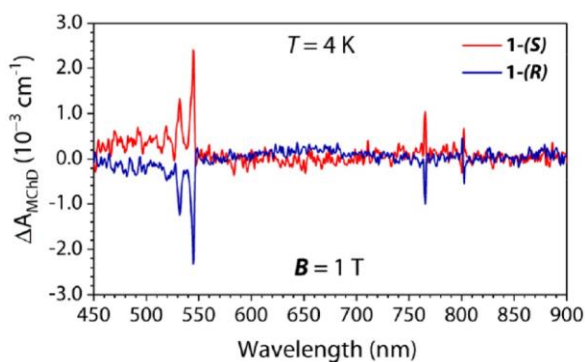
Cyrille Train,<sup>1</sup> Matteo Atzori,<sup>1</sup> Geert Rikken,<sup>1</sup> Maria Sara Raju<sup>1</sup>

<sup>1</sup> Laboratoire National des Champs Magnétiques Intenses (LNCMI), Univ. Grenoble Alpes, INSA Toulouse, Univ. Toulouse Paul Sabatier, EMFL, CNRS, Grenoble, France (email: [cyrille.train@lncmi.cnrs.fr](mailto:cyrille.train@lncmi.cnrs.fr))

Implementing chirality into magnetic systems is an open door towards materials exhibiting original properties. MagnetoChiral Dichroism (MChD) is one of these fascinating properties. It derives from a differential absorption of light going through a chiral AND magnetized medium. First discovered by G. Rikken<sup>(1)</sup>, it was then measured in oxalate-based bimetallic magnet under its Curie temperature,<sup>(2)</sup> establishing the proof-of-concept that this effect could be used for the optical readout of magnetic data using unpolarized light.



$P2_12_12_1$



A chiral Prussian Blue Analog exhibits magneto-chiral dichroism below its Curie Temperature.

Recently, thorough studies were conducted to establish the microscopic parameters driving this effect.<sup>(3-5)</sup> Spin-orbit being the most crucial ingredient to favor the intensity of MChD, we turned ourselves towards lanthanide-based systems.<sup>(6,7)</sup> The Yb(III) derivatives indeed exhibit very intense MChD response. Despite a weaker MChD response, Dy(III) derivatives, the most versatile complexes towards SMM properties, appeared as unavoidable candidates to try and probe SMM using MChD to extent the proof-of-concept once established for molecule-based magnets.<sup>(2)</sup> We indeed obtained promising results in this direction.<sup>(8)</sup>

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## Coordination Network-based Glasses: A new frontier of emerging materials

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Human civilization began producing traditional synthetic glass materials over 4,000 years ago. Since then, glass has become an essential part of daily life in human society. It is used in a wide range of applications, from everyday items like windows and drinking vessels to advanced technologies such as optical lenses and glass fibers for communication.[1] Recently, Coordination Network (CN)-based glasses have emerged as a new family of glass-forming materials. These network materials are composed of inorganic metal nodes and organic linkers. While most CNs decompose when heated, a few can melt at high temperatures and transition into glass through a process called vitrification. This discovery opens new avenues for innovation in glass materials. Lately, the focus has been shifted from the traditional glass preparation method of melt-quenching to the more modern approach of mechanochemical synthesis. The mechanochemical process offers several advantages over the melt-quench method for preparing glass materials. It requires less energy, operates under milder conditions, and is more environmentally friendly. This method also preserves sensitive materials that may decompose under high heat, allows for greater versatility in material composition, and can be accomplished more quickly. It is often more cost-efficient and easier to scale than traditional glass-making processes. Recently, we investigated a variety of CNs ranging from 1D to 3D structures with different  $d^{10}$  metal ions ( $\text{Ag}^+$ ,  $\text{Au}^+$ ,  $\text{Cu}^+$ ,  $\text{Pb}^{2+}$ , and  $\text{Zn}^{2+}$ ) coordinated through diverse organic linkers (such as nitriles, thiols, imidazoles, and amines).[2,3,4,5] The mechanochemical approach transformed these crystalline CNs into glasses, suitable for specific applications, such as photoluminescence[2,3,4] and gas uptake/storage[5].

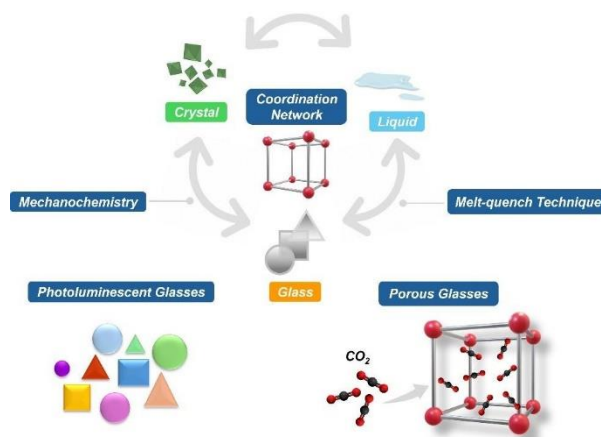


Figure 1. Schematic illustration of glass formation, and its application in photoluminescence and  $\text{CO}_2$  gas storage.

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## Design of H-bonded supramolecular Fe(II) switchable magnetic materials

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G. Rodríguez,<sup>a</sup> F. Trepard,<sup>a</sup> O. Roubeau,<sup>d</sup> G. Aromí<sup>a,b</sup>

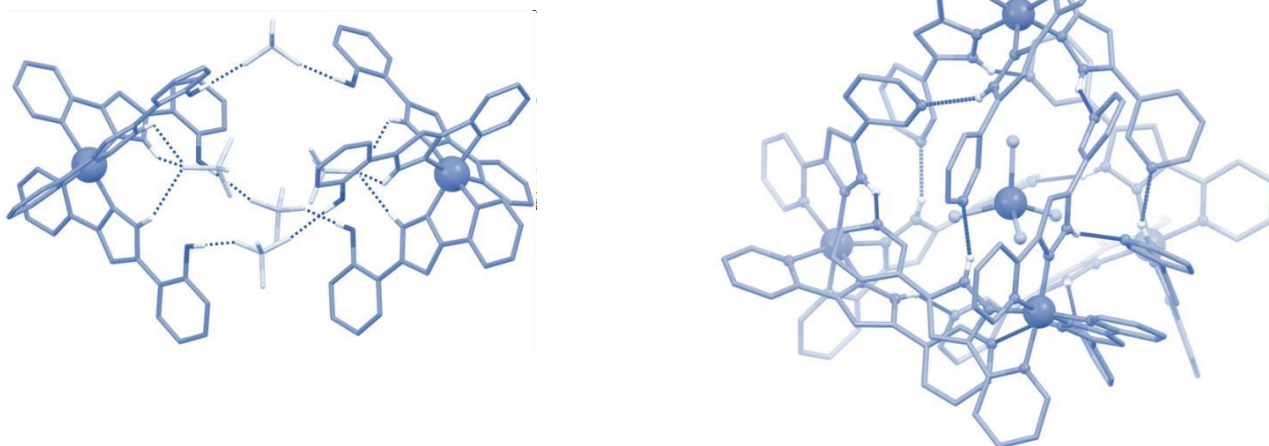
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Spin-Crossover (SCO) materials are fascinating switchable systems with great potential for the development of novel technological devices. Interestingly, their physical properties might be tuned by modifying weak non-covalent interactions, such as hydrogen bonds. In order to explore the potential of H-bonded SCO materials, we have designed ligands that combine a pyrazolylpyridyl chelating unit together with additional H-donor and/or acceptor groups.<sup>1,2</sup> The corresponding Fe(II) SCO compounds have been exploited to generate novel supramolecular architectures through H-bonding interactions (Figure 1) inducing concomitantly novel magnetic properties and evidencing the potential of this methodology to produce new switchable materials.



**Figure 1.** A supramolecular SCO anion-assisted helicate (left) and tetrahedron (right) produced by H-bonding interactions.

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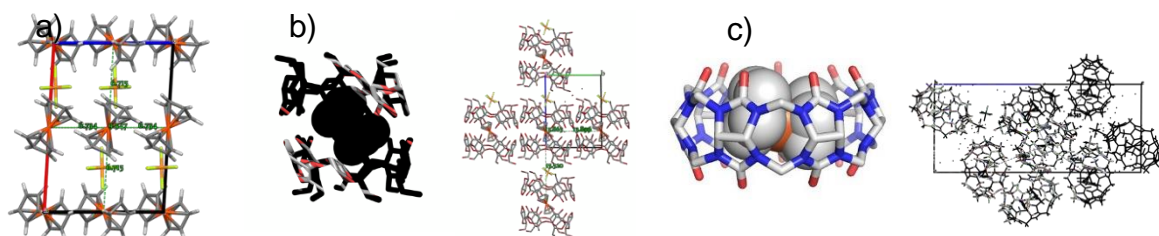
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## Insights into Single Molecule Magnets, from Blocking temperature to improving spin relaxation by encapsulation

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Magnetic molecules, and in particular Single-molecule magnets (SMM), have gained significant attention due to their potential use in technological devices, molecular spintronics, quantum computing and quantum sensing.<sup>1</sup> Their behavior is determined by the intrinsic magnetic anisotropy of the molecule and by the different mechanisms that allow the spin to relax and lose its coherence. Herein we highlight some of our recent work on SMMs. We present a general relation between the magnetization blocking temperature (TB),<sup>2</sup> one of the main characteristics of SMMs, measured using the zero-field cooling/field cooling technique (ZFC/FC) and their temperature-dependent spin relaxation time obtained from ac-susceptibility and magnetization decay measurements. Moreover, we showcase how the spin relaxation processes can be affected by its surroundings. The encapsulation of the previously studied ferrocenium cation<sup>3</sup> in different organic hosts a molecules, Figure 1, leads to an improvement of their magnetic properties.



**Figure 1** Views of the crystal structure of (a)  $[\text{FeCp}_2]\text{PF}_6$ , and encapsulated in (b)  $\alpha$ -cyclodextrin (1:2) and (c) cucurbit[7]uril (1:1). Iron, oxygen and carbon are shown in orange, red and grey respectively and hydrogens have been omitted for clarity.

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# Molecular Spin Qubits toward Quantum Computer and High-Density Memory Devices Based on Molecular Magnets

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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,  $\psi = a|0\rangle + b|1\rangle$ . 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  $S=1/2$ .

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**; To compare 0D [VO(TPP)] and 3D [VO(TCPP-Zn<sub>2</sub>-bpy)] (3D-MOF) to investigate the influence of the spin-lattice relaxation ( $T_1$ ) in 0D and 3D 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**; To compare [VO(TPP) and [CrN(TPP)] to investigate 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 short life time. **(3) Orbital Engineering Method**; To compare [Ni(cyclam)X<sub>2</sub>]ClO<sub>4</sub> and TBA[Ni(mnt)<sub>2</sub>] to investigate the relationship between the different occupied orbitals and spin relaxation. [Ni(cyclam)(NO<sub>3</sub>)<sub>2</sub>]ClO<sub>4</sub> has the longer life time due to the rigid molecular structure.

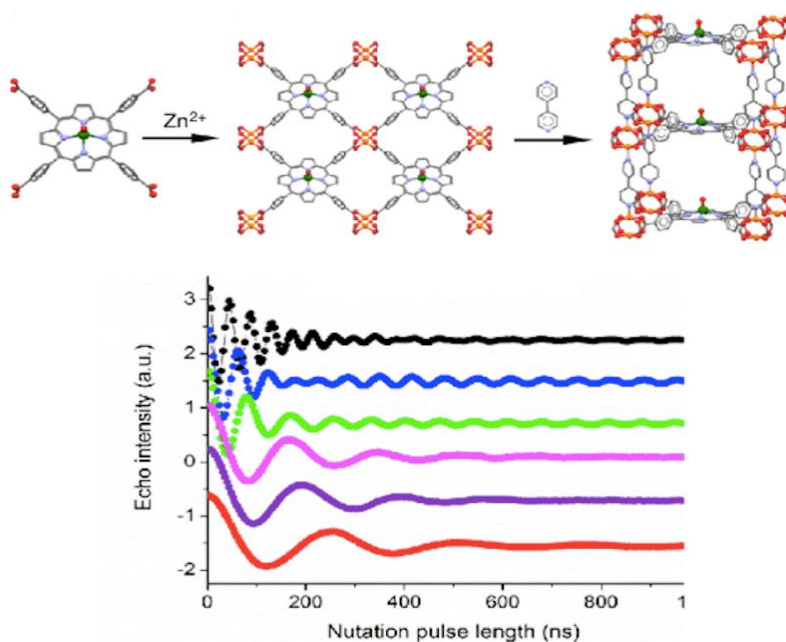
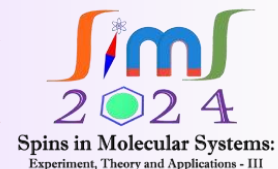


Fig.1. 3D MOF from 0D VO(TCPP) and Rabi Nutation at room temperature.





## Exact and approximate theory methods for quantum spin systems

Jürgen Schnack, Bielefeld University, Bielefeld, Germany

In this presentation I will demonstrate how modern theory methods help us to deal with very large quantum spin systems. In particular, I will focus on the use of symmetries as well as on very powerful approximate Krylov-space methods. This enables us to rationalize e.g. the magnetocaloric properties of a recently synthesized  $\{Gd_{12}Na_6\}$  molecular quadruple-wheel [1] or to discuss toroidal magnetic moments [2]. In an outlook I will show how spin systems are employed to study fundamental questions of thermalization in quantum mechanics, which for instance led to the discovery of synchronization phenomena [3].

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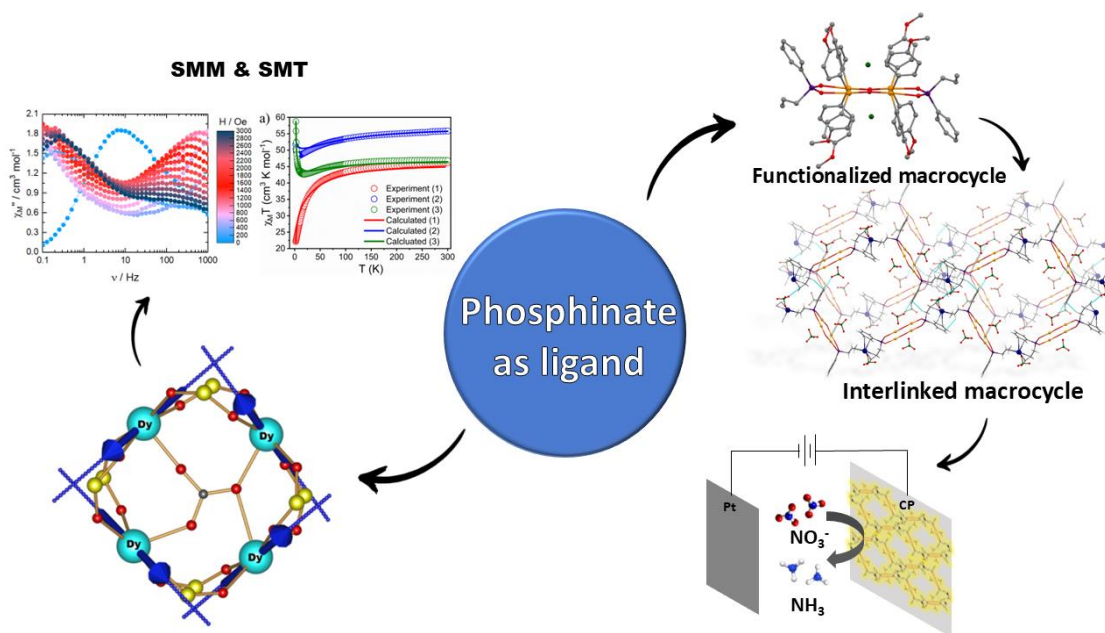
# Phosphinates for assembling molecular squares behaving as SMM/SMTs and Organometallic-Inorganic Hybrid Material acting as an Electrocatalyst

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Abstract: Phosphinates as ligands for assembling Ln clusters are quite rare when compared with carboxylates / phosphonates. Herein, we have used a phosphinic acid in assembling Ln clusters; SCXRD studies revealed the formation of Ln<sub>4</sub> (Er, Dy, and Tb) based molecular squares. Magnetic studies on these clusters revealed SMM (for Dy) and SMT (for Dy and Tb) behavior.<sup>1</sup> Further, we have functionalized phosphinates and have synthesized a 12-membered macrocycle on a diorganotellurium backbone. These macrocycles were interlinked to form 1D architectures by using metal- $\pi$  interaction. This hybrid material has been utilized as electrocatalyst for reduction of NO<sub>3</sub> to NH<sub>3</sub>.<sup>2</sup>



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## Gd(III)-based complexes as molecular spin qubits

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Qubits are the fundamental units of quantum information and computation. For successful quantum computing and information processing, qubits must meet several criteria, including having sufficiently long decoherence times. Among molecular spin qubits, most research has focused on ions with spin  $S = 1/2$ , which allow for the construction of single-qubit gates. However, qubits have to interact with each other for quantum operations, which has prompted research into molecules with  $S > 1/2$  and multilevel states.

In this communication, we report the study of the spin dynamics of a couple of mononuclear gadolinium-substituted polyoxometalate-organic hybrids namely  $K_5[Gd(\alpha-XW_{11}O_{39})(H_2L)] \cdot \sim 14H_2O$  ( $X = Si, Ge$ ;  $H_2L = N,N'$ -dimethyl- $N,N'$ -bis(2-hydroxy-3-formyl-5-bromobenzyl)ethylenediamine)<sup>1,2</sup> and we demonstrate the possibility to coherently manipulate their spin states. Pulsed EPR measurements reveal spin-lattice relaxation ( $T_1$ ) and quantum coherence ( $T_m$ ) times of up to 2315  $\mu s$  and 2.5  $\mu s$  at 3 K, respectively, for diamagnetically diluted samples, as well as Rabi oscillations up to 20 K.

### Acknowledgements:

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## Emphanisis: Local off-centering of atoms with warming

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Typical non-topological structural phase transitions involve an increase in crystal symmetry with rising temperatures. However, recent studies report an opposite trend in rare solid-state materials, where local symmetry decreases upon warming, a phenomenon termed as “*emphanisis*”. Despite being first evidenced in PbTe over a decade ago, the validity, specific chemical design elements, and underlying driving forces that predispose systems to exhibit *emphanisis* remain inconclusive. From a thermodynamic standpoint, it can be speculated that a phase may exhibit *emphanisis* if its free energy in its ordered undistorted state is lower than in its ordered distorted state, and the system can host a disordered distorted state upon warming. At low temperatures, the system adopts the ordered undistorted phase, while at higher temperatures, due to entropic stabilization, it transitions to a disordered distorted state encompassing low symmetry motifs in a symmetric matrix (from configurational averaging). Since these low-symmetry motifs can act as intrinsic phonon scatterers, engineering local-symmetry breaking through *emphanisis* is a promising strategy for realizing intrinsically ultralow lattice thermal conductivity in crystalline solids.<sup>1</sup>

In my talk, I will present the realization of *emphanisis* in few metal chalcogenide<sup>2-3</sup> and all-inorganic halide perovskite systems,<sup>4</sup> along with its experimental verification using synchrotron X-ray pair distribution functional analysis. The discussion will focus on the thermodynamics and chemical design elements that influence *emphanisis* and highlight their implications for achieving ultralow lattice thermal conductivity in crystals.

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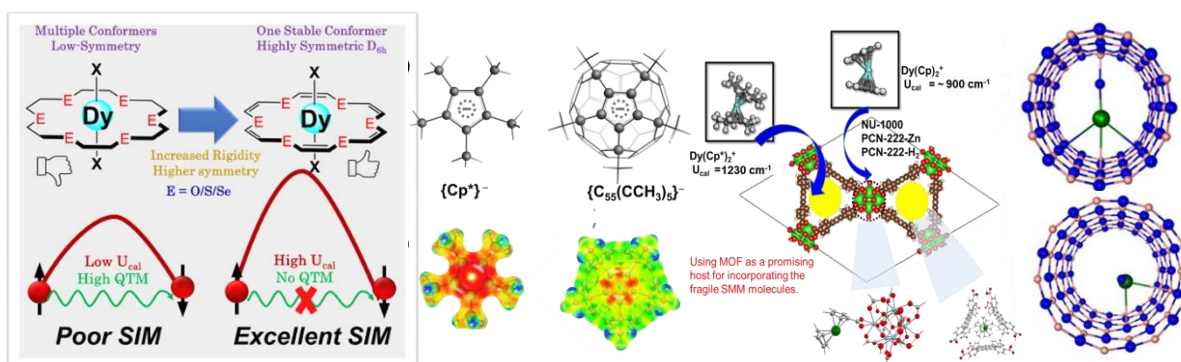
## Molecular Modelling of Ln(III) based Single-Ion Magnets and their Encapsulation in MOFs and Nanotubes

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Strongly anisotropic mononuclear lanthanide complexes are regarded as the best single-molecule magnets (SMMs) that display magnetic relaxation close to the boiling point of liquid nitrogen, opening up great potential for high-performance information storage, quantum information processing, and spintronic device applications.<sup>1</sup> In my presentation, I will discuss the application of ab initio-based ligand field theory (AILFT)<sup>2</sup> combined with multireference ab initio methods to investigate metal-ligand covalency and its significant role in fine-tuning the magnetic anisotropy of Dy(III) complexes. Here, I will describe the effect of ring size in organometallic sandwich complexes, inorganic ring sandwich complexes, and unsaturated thia crown ligands towards stabilizing highly anisotropic Dy(III) based SMMs. In the second part of my talk, I will describe the encapsulation of the  $[\text{DyCp}_2]^+$  cations and other highly anisotropic Dy(III) complexes in boron nitride nanotubes and metal-organic frameworks (MOFs) to shed light on the structure, energetics, magnetic anisotropy in hybrid assemblies.



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## New Insights into the Structural Chemistry of Doped Spin-Crossover Materials

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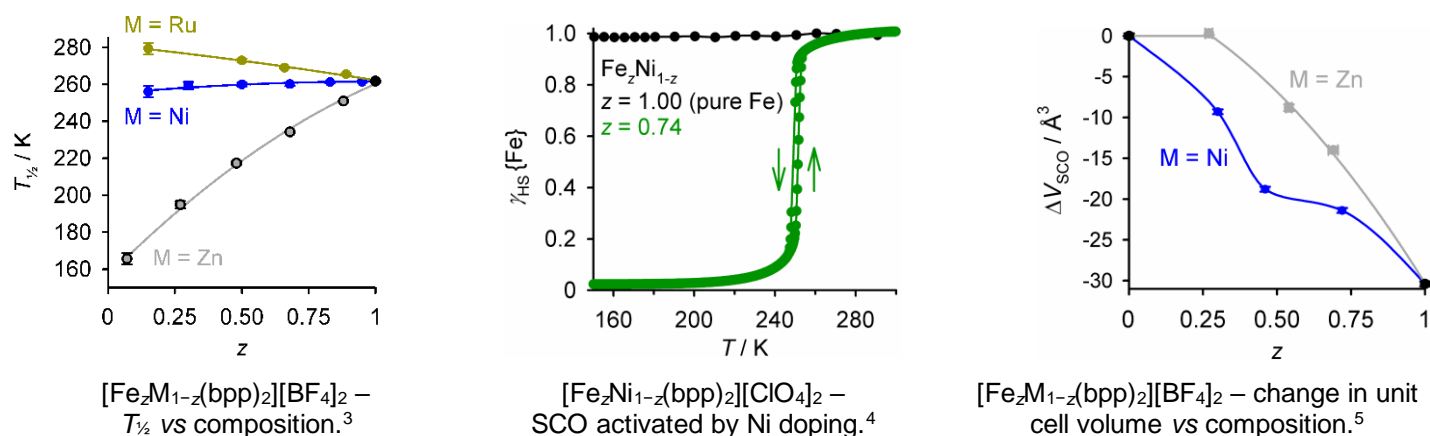
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Spin-crossover (SCO) materials treated with inert metal ion dopants are important probes of the lattice contribution to SCO thermodynamics and kinetics.<sup>1</sup> The temperature and form of SCO transitions in homogeneous solid solutions  $[\text{Fe}_x\text{M}_{1-x}\text{L}_n]^{m+}$  ( $\text{M}^{2+} = \text{Mn}^{2+}, \text{Co}^{2+}, \text{Ni}^{2+}, \text{Zn}^{2+}$  etc; L = a ligand;  $0 < x < 1$ ) changes systematically with dopant concentration, which is characteristic for different materials and dopants. This has led to a sophisticated understanding of lattice dynamics during SCO switching in macroscale and nanoscale materials, under thermodynamic and kinetic control.<sup>2</sup> We have used dopants to manipulate SCO functionality in other ways,<sup>3</sup> and this talk will describe our recent results from doped  $[\text{Fe}(\text{bpp})_2]^{2+}$  (bpp = 2,6-bis{pyrazol-1-yl}pyridine) complex salts:

- An unexpected result from doping  $[\text{Fe}(\text{bpp})_2][\text{BF}_4]_2$  with ruthenium(II);<sup>4</sup>
- Activating a high-spin compound to SCO using an inert molecular dopant;<sup>5</sup>
- Complicated structural changes during SCO in  $[\text{Fe}_z\text{M}_{1-z}(\text{bpp})_2][\text{BF}_4]_2$ .<sup>6</sup>



**Figure 1** Three results from doped SCO materials to be presented in this talk.

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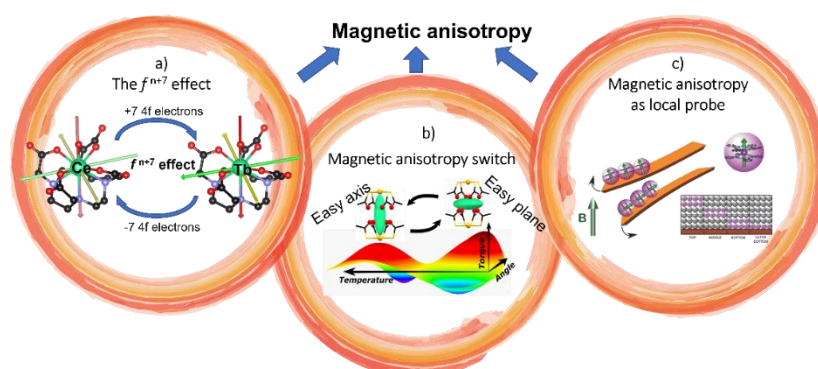
## Magnetic anisotropy: study, control and exploitation

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Magnetic anisotropy, i.e., the different magnetic response of a material depending on its orientation, is an important property in the field of quantum information [1]. Achieving a deep understanding and, ultimately, a full control over magnetic anisotropy is the key to design performant molecular magnetic materials such as Single Molecule Magnets, Magnetocaloric Agents or Pseudo Contact Shift Agents. In this talk, an overview of how magnetic anisotropy can be studied and exploited will be presented. Figure 1 shows three studies that will be highlighted: a) the  $f^{n+7}$  effect, i.e., the correspondence of magnetic reference frames between isostructural complexes differing by 7 4f-electrons [2], b) the use of external parameters such a temperature and magnetic field to manipulate the magnetic anisotropy, even on the surface [3,4] and c) how to probe molecular order on surface by exploiting magnetic anisotropy [5].



**Figure 1:** Figure 1. a) The  $f^{n+7}$  effect [2]. b) Magnetic anisotropy switch on a lanthanide complex [3,4] c) Molecular order on surface probed by torque magnetometry [5].

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Acknowledgments:

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## Detection of Magnetism in 2D via Dielectric Measurement

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Multifunctional devices based on spin-charge coupling involve low-frequency shifts of dielectric constant with magnetic ordering. Additionally, the presence of the magnetic anisotropy (MA) may drive the exotic spin textures and, in turn, lead to electric field control of the magnetic ground state [1]. Two-dimensional (2D) van der Waals (vdW) magnetic materials are of particular interest due to the presence of MA originating from the interaction between the magnetic moments and the crystal field [2-4]. We report anisotropic magnetodielectric coupling in layered van der Waals antiferromagnetic FePS<sub>3</sub> ( $T_N \sim 120$  K) with perpendicular anisotropy [1]. Above  $T_N$ , while the dielectric response function along the c axis shows frequency-dependent relaxations, in-plane data is frequency independent and reveals a deviation from phonon-anharmonicity in the ordered state, thereby implying a connection to spin-phonon coupling known to be indicative of onset of magnetic ordering. At low temperature (below 40 K), atypical anomaly in the dielectric constant is corroborated with temperature-dependent dc and ac susceptibility. The magnetodielectric response across this anomaly differs significantly for both in-plane and out-of-plane cases. We have explained this in terms of preferential orientation of magnetic antiferromagnetic zigzag alignment, implied by the in-plane structural anisotropy as confirmed by ab initio calculations. Controlling the relative strength of magnetodielectric coupling with magnetic anisotropy opens a strategy for tracking subtle modifications of structures, such as in-plane anisotropy, with potential applications for spintronic technologies.

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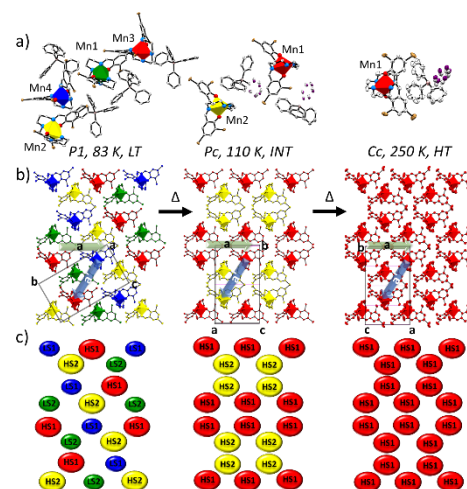
## Spin State Ordering and Domain Wall Dynamics in Magnetoelectric Spin Crossover Materials

G. Morgan,<sup>\*a</sup> V. Jakobsen,<sup>a</sup> H. Müller-Bunz,<sup>a</sup> E. Trzop,<sup>b</sup> V. Zapf,<sup>c</sup> M. Carpenter,<sup>d</sup> E. Collet<sup>b</sup>

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Domain walls (DWs) in ferroic materials – ferromagnets, ferroelectrics, ferroelastics - represent the regions where there is a change in order parameter. Here we report domain wall motion in a molecular system during the transition to a ferroelastic and spin-state ordered phase of a spin crossover complex. Single crystal X-ray diffraction,  $\mu$ SR and resonant ultrasonic spectroscopy (RUS) were used to detect a variety of symmetry-breaking phase transitions in the mononuclear  $Mn^{3+}$  compounds  $[Mn(3,5\text{-diBr-sal}_2(323))]BPh_4$ , (**1**) and  $[Mn(3,5\text{-diCl-sal}_2(323))]BPh_4$  (**2**).<sup>[1],[2]</sup> These involve continuous ( $Cc \rightarrow Pc$ ) and discontinuous ( $Pc \rightarrow P1$ ) space group changes and stress-induced domain wall mobility was detected as softening of the phonon modes at the  $Pc \rightarrow P1$  transition in both cases. We compare the electric polarization change that accompanies the spin crossover for (**1**) and (**2**) which remains trapped after the magnetic field is removed in both cases.<sup>[2],[3]</sup> Thus we demonstrate a route to magnetic field-switchable electric polarization at a spin state transition in molecular systems.



**Figure 1** View of the LT P1 (83 K), INT Pc (110 K) and HT Cc (250 K) structures of complex 1.

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## Redox Mediated Synthesis of Main-Group Based Open-Shell Compounds

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In molecular chemistry, the redox (reduction/oxidation) processes are crucial for various synthetic transformations. At the same time, open-shell compounds (those having half-filled orbital(s)!) are very important for various purposes, from their application in synthetic chemistry to advanced materials such as high-spin molecular systems. The molecules must contain electron-donor and/or electron-acceptor motif(s) to participate in redox reactions. Therefore, by designing judicious redox reactions, it is possible to create various classes of open-shell compounds by controlling the injection or removal of a particular number of electrons at the redox-active motif(s) and resulting in the center(s) of an odd number of electrons(s).

In this talk, I shall discuss the effort of our research group in designing and developing convenient modular routes for synthesizing compounds that contain mono-/bis-alkenes as electron-donor motifs<sup>1</sup> and mono-/bis-cyclic/acyclic carbocations/iminium cations along with boranes/boryl-cations as electron-acceptor motifs,<sup>2</sup> subsequently its utilization as synthons for isolating various open-shell compounds: radicals, radical-cations, (cationic)-diradicals, radical-trications, and (cationic/heteronuclear)-diradicaloids under redox (reduction/oxidation) reaction conditions will be elaborated.<sup>3</sup> Moreover, I shall discuss the pivotal role of the spin-carriers and spin-couplers in the resulting electronic situation of the open-shell molecules.

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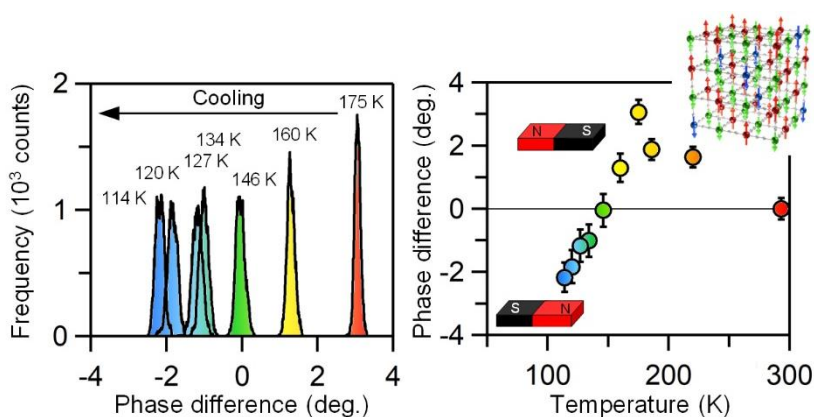
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## Study of Magnetic Domains in Magnetization Reversal on FeCr-hexacyanide magnetic film

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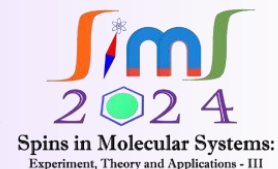
In molecule-based magnets, one can design magnetic properties, such as saturation magnetization, Curie temperature ( $T_C$ ), and coercive field, by selecting metal ions, radicals, and incorporated ligands. Herein, we study the magnetic domains of molecule-based magnets.<sup>1</sup> As target materials, two hexacyano-iron-chromate  $\text{Fe}_x\text{Cr}_{1-x}[\text{Cr}(\text{CN})_6]_{2/3} \cdot 5\text{H}_2\text{O}$  films ( $x = 0$ ; **Film 1** and  $x = 0.2$ ; **Film 2**) were prepared. The surface-magnetized states were measured using magnetic force microscopy. **Film 1** shows magnetic domain below  $T_C$  with a maze pattern. In **Film 2**, positive magnetic polarization appears below  $T_C$ , and magnetization becomes zero at a particular temperature ( $T_p = 146$  K), changing magnetic polarization to negative. Monte Carlo calculations implied that  $T_p$  is the compensation temperature. A direct observation of temperature-variable behaviour of compensation temperature has not been previously reported. This study can progress molecule-based magnets from magnetochemistry to magnetostatic engineering of bulk magnets, thereby opening a new field of molecule-based magnetostatic engineering.



**Figure 1** Film 2 shows positive magnetic polarization below  $T_C$ , and the magnetization becomes zero at a particular temperature, changing the magnetic polarization to negative.

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## "Electron Diffraction – An Innovative and Advantageous Tool for Structure Determination of Nanocrystalline Materials"

- Dr. Alessia Portieri from ELDICO Scientific AG.

*Electron Diffraction (or 3DED, ED, MicroED) is emerging as a powerful technique for the structural elucidation of challenging compounds as it bypasses the main limitation of growing crystals of suitable size for single-crystal X-ray diffraction. Applications range from natural products and pharmacology to geological sciences, advanced materials, nanotechnology, and many more. MicroED is also merging in the crystallographic community due to its incredible advantages that combine X-Ray benefits with Electron Microscopy. By combining the imaging features (STEM mode) with the diffraction mode of an electron diffractometer, crystal mapping of dozens to hundreds of nanosized single crystals can provide the missing information needed to fully understand the PXRD profiles. Electron Diffraction opens new innovative applications for people working in the industry and academic world for applications like impurity profiling, detecting micro crystallinity in amorphous materials, assisted solid state screening, which no other technology can do at this moment as swift and accurate. In this talk Dr. Alessia Portieri, ELDICO Scientific AG, Switzerland, will show a range of examples including both nanocrystalline samples of known MOFs and new materials, all measured in continuous rotation mode on a dedicated electron diffractometer. The results illustrate the potential of this technique in the field of porous coordination networks and the benefits of dedicated instrumentation that has become available in recent years.*



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**MODERN TRENDS IN MOLECULAR MAGNETISM – IV**  
**&**  
**SPINS IN MOLECULAR SYSTEMS:**  
**EXPERIMENT, THEORY AND APPLICATIONS – III**



**Alex Melville (Cryogenics)**



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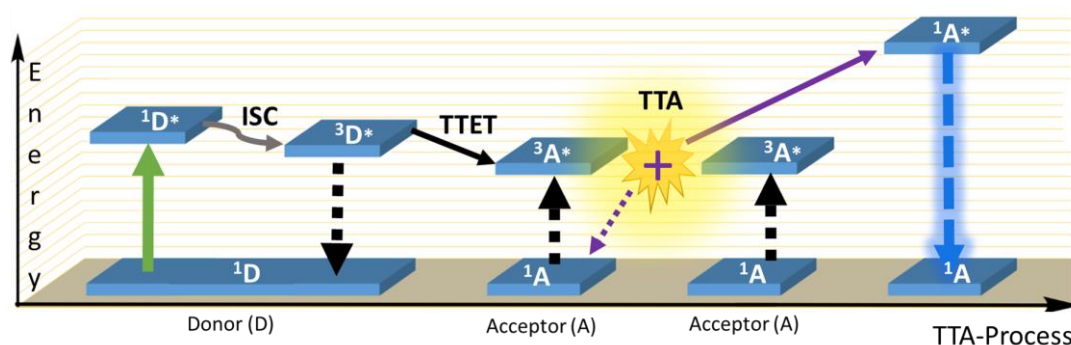
## Triplet-Triplet Annihilation-based Photochemical Photon Upconversion of Low Intensity Light

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In photochemical upconversion processes, the released light contains photons that are higher in energy than the absorbed ones. There are various other methods that may produce energy upconverted photons, such as two (or multi) photon absorption (TPA), second harmonic generation (SHG), etc., however, they require very powerful energy sources ( $\sim \text{GW}/\text{cm}^2$ ). Low intensity light such as sun light cannot be upconverted through these methods. This limitation could be overcome by applying triplet-triplet annihilation-based photon upconversion (TTA-UC), which can take place under much milder conditions ( $\sim \text{mW}/\text{cm}^2$ ).<sup>1, 2</sup> Materials capable of TTA-UC find numerous applications in light-based devices and in the field of theranostics.<sup>3-6</sup> TTA-UC process (Figure 1) depends largely on generation, triplet energy transfer and triplet annihilation steps. In this talk, I will discuss about the various methodologies that may be adopted to protect the triplets and to maximize the upconversion quantum yields.



**Figure 1:** Schematic diagram showing steps involved in TTA-UC.

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**MODERN TRENDS IN MOLECULAR MAGNETISM – IV  
&  
SPINS IN MOLECULAR SYSTEMS:  
EXPERIMENT, THEORY AND APPLICATIONS – III**



**Horiba**



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## Giving Chemistry Direction

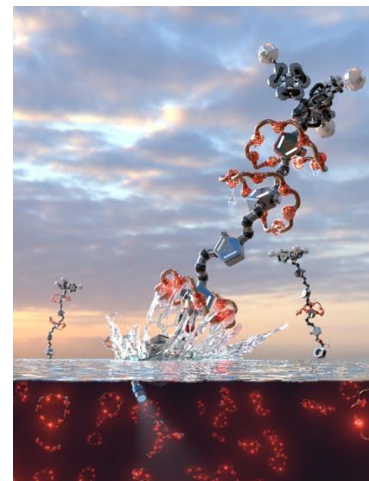
Prof David A. Leigh

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Over the last three decades examples of synthetic molecular machines and motors<sup>1</sup> have been developed,<sup>2</sup> all be they primitive by biological standards. Such molecules are best designed to work through statistical mechanisms.<sup>3</sup> In a manner reminiscent of Maxwell's Demon,<sup>4</sup> random thermal motion is rectified through ratchet mechanisms,<sup>3-9</sup> giving chemistry direction.

It is increasingly being recognised that similar concepts can be applied to other chemical exchange processes.<sup>10</sup> Ratchet mechanisms—effectively chemical engines<sup>11</sup> in which catalysis<sup>5,7,8</sup> of 'fuel' to 'waste' is used to drive another chemical process—can cause directional impetus in what are otherwise stochastic systems, including endergonic chemical reactions<sup>12</sup>. This is ushering in a new era of non-equilibrium chemistry, providing fundamental advances in functional molecule design and the first examples of molecular robotics,<sup>13,14</sup> overturning existing dogma and offering fresh insights into biology and molecular nanotechnology.



For a musical introduction, see 'Nanobot': <https://bit.ly/2M5Zwdl>

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## Assembling Prussian Blue Analogs Using Hydrogen Bond-Donating Unit toward Complete Phase Transition

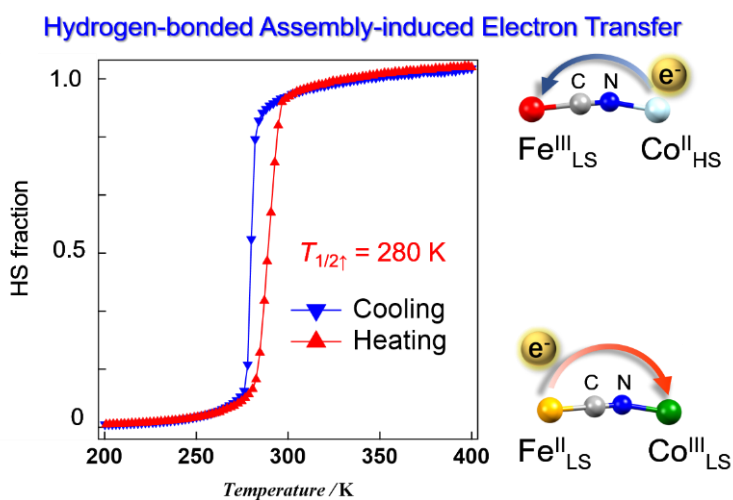
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The exploration of new functional compounds based on coordination chemistry is an important subject in the field of materials science. Finely tuning structure, electronic, and spin states in molecular materials, namely flexible charge/spin compounds, is an attractive theme for developing external stimuli-responsive coordination metal complex-based materials.<sup>[1-3]</sup> Thermally driven electron transfer systems are a class of “smart” and “frontier” materials among such material systems that lead not only to change their oxidation states but also their electronic states, enabling switching of physical properties. Cyano-bridged polynuclear metal complexes exhibit unique electronic and magnetic properties.



This presentation demonstrated the synthesis of new Co/Fe complexes for exploring external stimuli-responsive materials. After self-assembling **1** (non-responsive complex) with hydrogen-bonding donor molecules, the supramolecular assembly **2** was successfully constructed. Temperature-dependent structural analyses for **2** revealed that the coordination bond distances around metal ions are significantly changed due to the electron

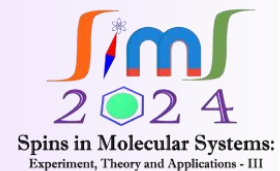
transfer occurrences.<sup>[4]</sup> Consequently, we have demonstrated a new strategy for complete phase transition behavior using the hydrogen assembly method. Crystal engineering of hydrogen-bonded architecture can influence their packing motif and electronic state variation, yielded in the fine-tuning of the electron transfers.

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**MODERN TRENDS IN MOLECULAR MAGNETISM – IV  
&  
SPINS IN MOLECULAR SYSTEMS:  
EXPERIMENT, THEORY AND APPLICATIONS – III**



**Guillem Aromi**



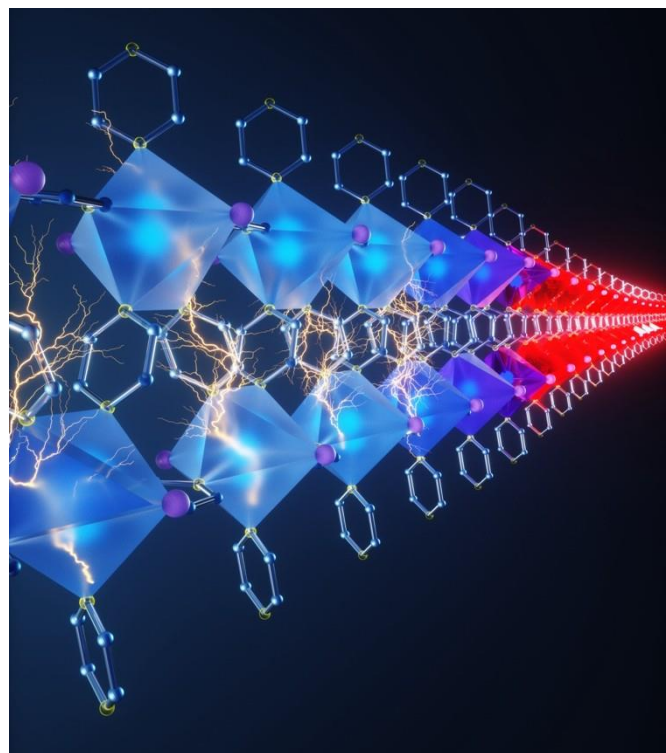
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## Molecular Mosaics Losing Their Innocence

Kasper S. Pedersen

Department of Chemistry, Technical University of Denmark

Quantum materials exhibit exotic phenomena arising from the intricate interplay between electronic, magnetic, and lattice degrees of freedom. Virtually all quantum materials are inorganic in nature and synthesized under conditions that provide nothing but thermodynamic control as a synthetic handle. Molecular chemistry offers the tools for addressing contemporary problems in quantum materials discovery, enabling the rational design, synthesis, characterization, and understanding of novel materials. Metal-ligand assemblies with variable or hardly separable valences (“non-innocence”) are pervasive in molecular coordination chemistry and host the possibility to tame strong electron-electron correlations in extended networks, thereby representing a realistic strategy to challenge current state-of-the-art in quantum materials



discovery. The use of well-defined metal ion “building blocks” with predictable bonding characteristics as nodes, in conjunction with rigid molecular linkers, provides a novel strategy to synthetically tailor materials’ tessellations. In the lecture I will discuss the group’s recent findings in the quest for genuinely new symmetries and properties in metal-organic framework materials and showcase how the use of novel 3D electron diffraction methods applied in our laboratory will accelerate materials discovery, broadly defined.

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## Electron Transport Through Perfect 1D Atomic/Molecular Chains

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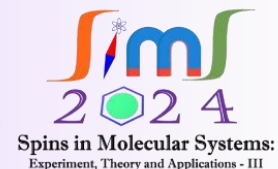
Creating an environmentally stable highly transmitting metal/molecular/metal junction via resonant transport at ambient condition is one of the key challenges in the field of molecular electronics. The necessary requirement for achieving such a resonant transport is to align the metal Fermi level with one of the frontier orbitals of the molecule. A molecule connected between two metal electrodes serves as the basic building block for studying electron transport at this atomic/molecular scale. Experimentally it can be achieved by using the break junction technique. In this talk, I will discuss transport phenomena in two different molecular junctions. Firstly, I will show results from Au-Ferrocene single molecular junction, where we observe a formation of stable conducting junction at room temperature with a significantly high conductance of  $\sim 0.2 \cdot 2e^2/h$ ,  $h$  being the Plank's constant. Transport calculations in the molecular junctions show significant transmission in the vertical geometry with metal-Fe-metal bond formation, leading to high conductance. The temperature dependent transport reveals interesting features which has a direct correlation with the dynamic structure of the molecule. We also showed that the electronic transport of these junctions can be manipulated via mechanical gating, and it is indeed sensitive to the orientation of the molecule. Finally, I will discuss the formation and evolution of a perfect one-dimensional atomic chain assisted by molecules.

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3. Machine-learning prediction on formation of atomic gold wires by mechanically controlled break junction, Aishwaryo Ghosh#, Biswajit Pabi#, Atindra Nath Pal\* and Tanusri Saha-Dasgupta\*, **Nanoscale** 15 (42), 17045-17054 (2023). (# equal contributions)
4. Unusual electro-mechanical response in a Ferrocene-assisted gold atomic chain, Biswajit Pabi et al., (under preparation).



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## COUPLING MAGNETISM TO ELECTRICITY IN MULTIFERROIC HETEROSTRUCTURES

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Complex perovskite oxides exhibit a rich spectrum of functional responses, including magnetism, ferroelectricity, highly correlated electron behavior, superconductivity, etc. The basic materials physics of such materials provide the ideal playground for interdisciplinary scientific exploration. Over the past decade we have been exploring the science of such materials (for example, colossal magnetoresistance, ferroelectricity, etc) in thin film form by creating epitaxial heterostructures and nanostructures. Among the large number of materials systems, there exists a small set of materials which exhibit multiple order parameters; these are known as multiferroics. Using our work in the field of ferroelectric(FE) and ferromagnetic oxides as the background, we are now exploring such materials, as epitaxial thin films as well as nanostructures. Specifically, we are studying the role of thin film growth, heteroepitaxy and processing on the basic properties as well as magnitude of the coupling between the order parameters. In our work we are exploring the switchability of the antiferromagnetic order using this coupling.

What is the importance of this work ? Antiferromagnets(AFM) are pervasive in the recording industry. They are used as exchange biasing layers in MTJ's etc. However, to date there has been no antiferromagnet that is electrically tunable. We believe that the multiferroic BiFeO<sub>3</sub> is one compound where this can be observed at room temperature. The next step is to explore the coupling of a ferromagnet to this antiferromagnet through the exchange biasing concept. Ultimately, this will give us the opportunity to switch the magnetic state in a ferromagnet( and therefore the spin polarization direction) by simply applying an electric field to the underlying antiferromagnetic ferroelectric. In this talk, I will describe our progress to date on this exciting possibility.



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## Recent Advances in Actinide-Actinide Bonding: Trithorium Clusters

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Over the best part of two centuries molecular metal-metal bonding has become a mature field spanning numerous s-, p-, and d-block elements. In contrast, molecular compounds with actinide-actinide bonding remained exceedingly rare, with examples restricted to diatomics in cryogenic inert matrices, gas-phase spectroscopic transients, or encapsulated in endohedral fullerenes. Recently, we discovered that actinide-actinide bonding can be accessed in a trithorium cluster.<sup>1</sup> This complex is notable for being preparable on multi-gram scale and also because it exhibits unusual three-centre two-electron bonding unlike the traditional  $\sigma$ -/ $\pi$ -/ $\delta$ - bonding motifs commonly found with transition metals. This talk will discuss our ongoing work in the area.

We thank the Engineering and Physical Sciences Research Council, Natural Environment Research Council, Deutsche Forschungsgemeinschaft, European Research Council, Royal Society, National Nuclear Laboratory, Chinese Scholarship Council, University of Manchester (including the Computational Shared Facility), and University of Stuttgart, for generous support. The Alexander von Humboldt Foundation is thanked for a Friedrich Wilhelm Bessel Research Award to S.T.L.

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# Robust topological Hall effect in ultra-thin Cr<sub>2</sub>Te<sub>3</sub> films by Vanadyl phthalocyanine coupling

Karthik V. Raman, Suman Mundlia

Layered magnetic transition metal chalcogenides (TMDs) have been a hotbed of research, unveiling a plethora of exotic magnetic and topological phenomena. Among the material choices in TMDs, Cr<sub>2</sub>Te<sub>3</sub> has emerged as a promising candidate, drawing significant attention for its excellent tunability in magnetic response owing to competing exchange interactions. In this talk, we demonstrate the manipulation of magnetic anisotropy of ultra-thin Cr<sub>2</sub>Te<sub>3</sub> films through modulation of the Cr:Te flux ratio during our film deposition. This modulation leads to a remarkable transition in magnetic anisotropy from in-plane to out-of-plane orientation with an intermediate non-co-planar magnetic ground phase characterized by a topological Hall response. Moreover, interfacing these films with vanadyl phthalocyanine (VOPc) molecules prominently enhances the topological magnetic phase over a wider Cr:Te flux-ratio, stemming from modification in surface magnetic exchange interactions in Cr<sub>2</sub>Te<sub>3</sub> due to VOPc adsorption. Our findings pave the way for the realization of interface-modulated magnetic exchange coupling through molecular growth, offering exciting prospects for future research in this burgeoning field.

This work is supported by ONR Global, DAE Project Identification No. RTI 4007.



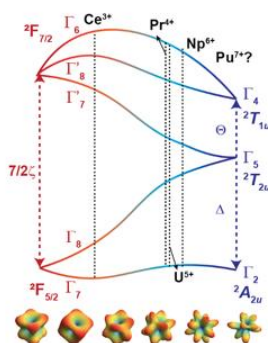
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# Static and dynamic magnetic properties of tetravalent lanthanide ions

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- Nuclear and Radiological Engineering and Medical Physics Program, School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332-0400, United States
- Physical Sciences Division, Pacific Northwest National Laboratory, Richland, Washington 99352, United States  
\*hsl@gatech.edu

Using a suite of spectroscopic and theoretical tools, this talk will discuss how in  $\text{Pr}^{4+}$ , with a  $4f^1$  valence electronic configuration, competition between spin-orbit coupling and crystal field interactions transforms the spin-orbital magnetism of the ion and departs from the  $j_{\text{eff}} = 1/2$  limit. This intermediate coupling regime (Figure 1), which in many ways resembles high-valent actinide ions, quenches orbital angular momentum and facilitates the ligand- field tuning of the spin-orbit coupled states of the  $\text{Pr}^{4+}$  ion.<sup>1</sup> In our study of the coherence properties of  $\text{Pr}^{4+}$ , we demonstrate that the anomalously large crystal field splitting of  $\text{Pr}^{4+}$  facilitates avoiding overlap of electronic excitations with the vibrational density of states.<sup>2</sup> If there is time, discussion of the extension of this model to magnetometric and EPR studies of molecular high-valent lanthanide ( $\text{Pr}^{4+}$  and  $\text{Tb}^{4+}$ ) complexes will be included.<sup>3,4</sup>



**Figure 1** Schematic of the splitting of  $f$  orbitals as a function of CF ( $\Delta$  and  $\theta$ ) relative to SOC ( $\zeta$ ).

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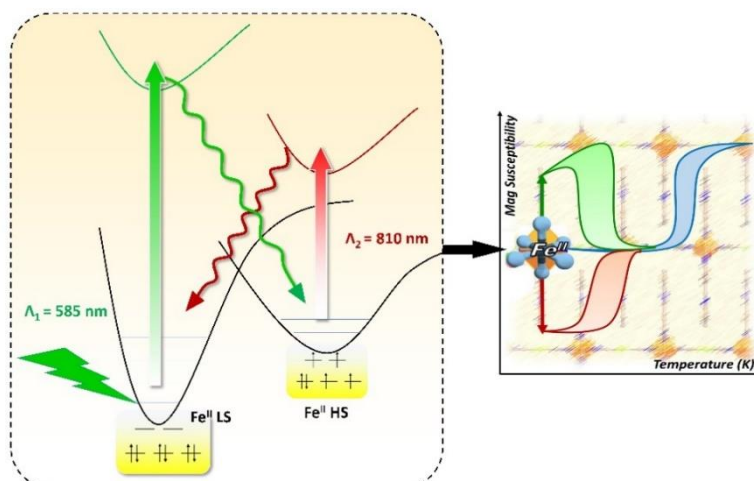
# Spin-State Switching in Dynamic Molecules and Chiral Cages

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The development of molecular materials that can be switched between two different spin states through the application of external stimuli is of great interest owing to their potential use in molecular devices and information technology<sup>[1,2]</sup>. 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. Some exciting recent discoveries<sup>[3-4]</sup> 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. In the second part, I will discuss the self-assembled enantioselective formation Fe(II) chiral cages, where, the guest molecules determines the chirality of the host system, by a relatively new approach known as "Reverse Chiral Recognition"<sup>[5]</sup>.



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International Conference on  
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## Speakers for Day 2 : 6<sup>th</sup> November 2024

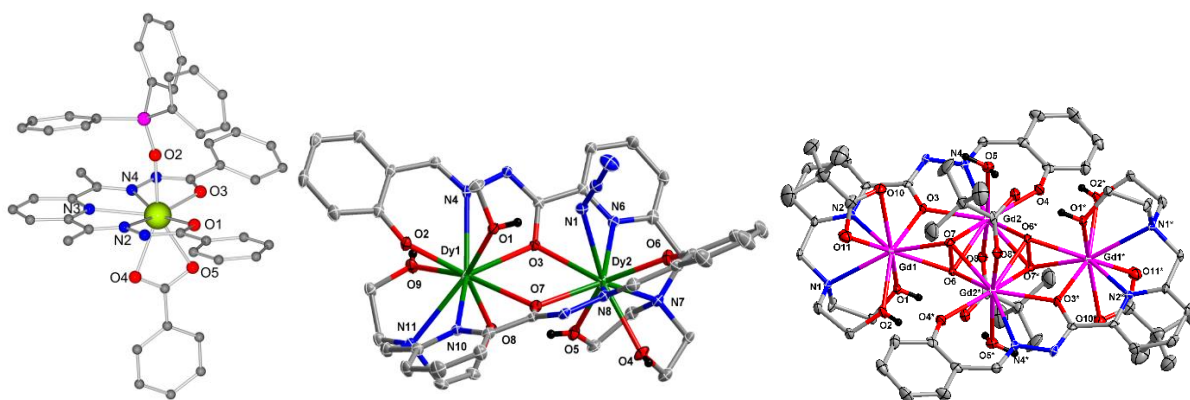
- 1) Vadapalli Chandrasekhar
- 2) Talal Mallah
- 3) Sankar P. Rath
- 4) Sally Brooker
- 5) Rodrigue Lescouëzec
- 6) Ravindra Venkatramani
- 7) Nicholas F. Chilton
- 8) Marius Andruh
- 9) R. Boomi Shankar
- 10) Siddhartha De (ERL)
- 11) Kehkasha Siddiqui (ERL)
- 12) S. M. Hossain (ERL)
- 13) Vijay Parmar (ERL)
- 14) Muralidharan Shanmugam
- 15) Arpan Mondal (ERL)
- 16) Deepanshu Chauhan (ERL)
- 17) Eric Collet
- 18) Somobrata Acharya
- 19) Satish Patil
- 20) Rémi Maurice
- 21) Osamu Sato
- 22) Lapo Bogani
- 23) Shouvik Chatterjee
- 24) Matthew J. Cliffe
- 25) Indra Dasgupta
- 26) Robert Podgajny
- 27) Mahesh Sundararajan
- 28) Swadhin Mandal
- 29) Nathalie Guihéry
- 30) Tharamani C. N
- 31) Abhishek Banerjee
- 32) Martin Lemaire
- 33) Narcis Avarvari
- 34) Kartik C. Mondal
- 35) Michael Shatruk
- 36) Athanassios K Boudalis
- 37) Phani K. Peddibhotla
- 38) Robert Baker
- 39) Shinya Hayami
- 40) Hélène Bolvin



# Synthetic Strategies for the Assembly of Mononuclear, Dinuclear and Tetranuclear Lanthanide Complexes

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In this talk we will present some synthetic strategies that allow a rational assembly of lanthanide complexes with varied nuclearity. Specifically, we will examine the synthesis of mono- di- and tetranuclear complexes (Figure 1). The ligand design and usefulness of specific ancillary ligands for the preparation of such complexes will be presented. The structural characterization and magnetic properties of these families of lanthanide complexes will also be discussed.



**Figure 1.** Molecular structures of representative examples of mononuclear (left), dinuclear (middle), and tetranuclear (right) lanthanide complexes.<sup>1-3</sup>

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## Magnetic molecules based on transition metal ions as spin quantum bits

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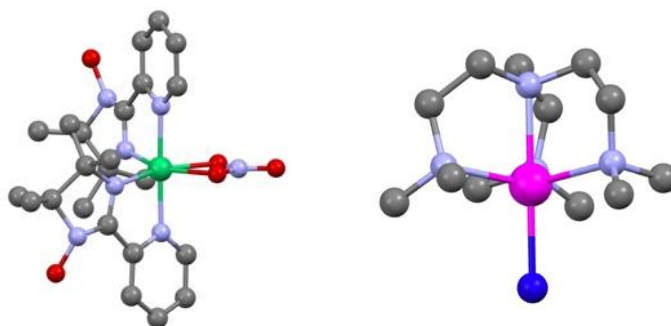
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The nature of the ligands (electronic effects) and the geometry of paramagnetic coordination complexes lift the degeneracy of the spin state sublevels (for  $S > \frac{1}{2}$ ) and leads to a low-lying two-level system (in the absence of external magnetic field for non-Kramers levels and in the presence of a magnetic field for Kramers doublets) that may behave as a spin quantum bits. This is the case of the two mononuclear complexes Ni(II) and Mn(II) whose structure is depicted in Figure 1. For Ni(II), calculations and Electron Paramagnetic Resonance (EPR) spectroscopy show that the  $M_S = \pm 1$  sublevels are lower in energy than  $M_S = 0$  ( $D = -10.5 \text{ cm}^{-1}$ ) and its degeneracy is lifted thanks to a slight rhombicity ( $E = 0.15 \text{ cm}^{-1}$ ). The gap ( $2E$ ) between that defines the qubit frequency is very close to the X-band microwave energy ( $0.32 \text{ cm}^{-1}$ ), so that a clock transition is expected at zero applied magnetic field. In this presentation, we show that, thanks to the clock transition at zero field, the coherence of the superposed state is well protected from the magnetic fluctuations of the spin bath. We also briefly discuss the effect of an electric field on the modulation of the electronic parameters characterizing the quantum bit in the case of half-integer spin mononuclear complexes (Mn(II),  $S = 5/2$ , Figure 1-right), with a view to electrically addressing quantum bits.



**Figure 1.** View of the structure of the mononuclear Ni(II) (left) and Mn(II) (right) complexes

# Metal vs. Ligand Oxidation: Electronic Communication through Bridge and Spin Coupling

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*MauG* is a terminal enzyme involved in the biosynthesis of the catalytic tryptophan tryptophenylquinone (TTQ) cofactor of methylamine dehydrogenase (MADH). Although two heme units are physically separated in the enzyme, they share electron efficiently behaving as a single diheme unit. A tryptophan residue, positioned midway between the heme centers, has been postulated to act as a bridge for electronic communications. Biomimetic studies of these systems provide valuable information regarding the mechanisms of electron and charge transport behaviors and provide promising platforms for systematic studies of spin coupling to promote long-range communication across the bridge connecting the metalloporphyrin centers. Interaction between the organic radical and paramagnetic metal centre is important machinery for designing functional magnetic materials with desired properties. The results will be highlighted in the talk.<sup>1-4</sup>

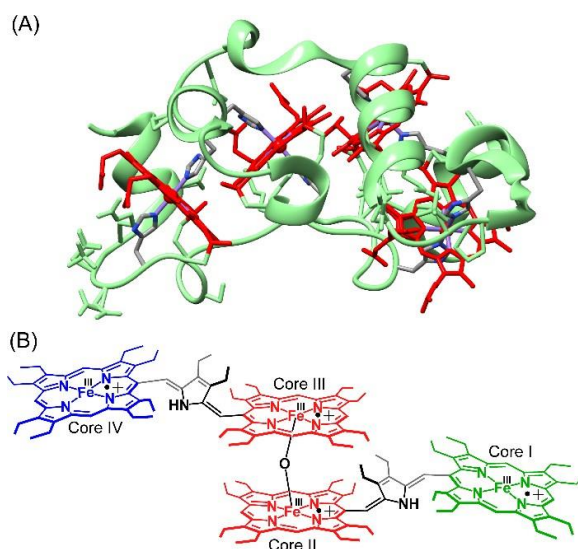


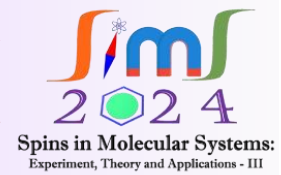
Figure 1. (A) Stereoview of small tetraheme cytochrome c isolated from *Shewanella Oneidensis* and (B) tetra-heme unit reported here (axial coordination and counter anions are not shown).

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**MODERN TRENDS IN MOLECULAR MAGNETISM – IV  
&  
SPINS IN MOLECULAR SYSTEMS:  
EXPERIMENT, THEORY AND APPLICATIONS – III**



Sally Brooker



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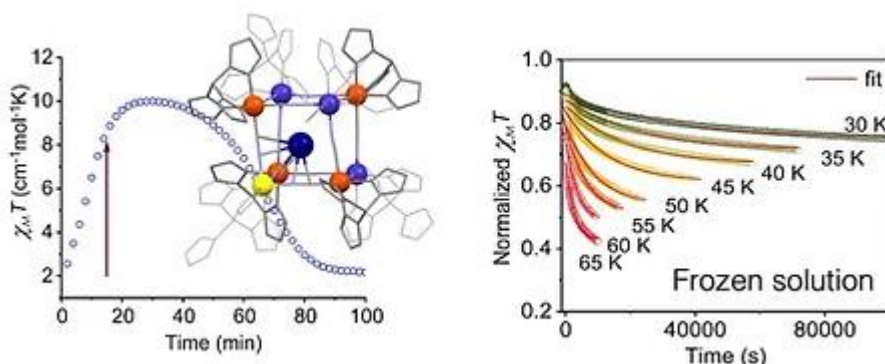
## Molecular Switches based on Metal-Metal Electron Transfer

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Molecular magnetic switches are molecules which undergo reversible conversions between two distinct electronic states under external stimuli: temperature, light, pressure. The change of electronic states can be associated to drastic modification in the magnetic properties but also in the optical, dielectric and mechanic properties. To date, the most investigated molecular magnetic switches are spin-crossover complexes (SCO). Another class of bistable magnetic compounds has emerged in which the electronic reorganization involved two cyanide-bridged neighboring metal ions. Here the electronic-state change often implies a metal-to-metal Electron Transfer Coupled to a Spin Transition on one metal ion (ETCST transition). The effect was first evidence in inorganic polymers (FeCo Prussian Blue Analogs) but strong research efforts have recently been devoted to the design of their discrete molecular analogs.

In this presentation, we will present some of our recent works that are either devoted to in-depth understanding of the switchable phenomena or to harness their utility as molecular sensors, actuators or memories in future technological applications.<sup>1-4</sup>



Photoinduced  $\text{Fe}^{\text{II}}\text{Co}^{\text{III}} \leftrightarrow \text{Fe}^{\text{III}}\text{Co}^{\text{II}}$  conversion in a  $\text{Fe}_4\text{Co}_4$  cubic complex (left: XT vs T curve after irradiation; right: isothermal relaxation of the photo-induced paramagnetic state)

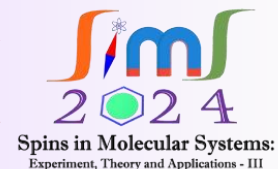
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## Electronic Molecular Breadboards

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I will present an original idea of molecular breadboards which can enable researchers to test and prototype combinations of electronic circuits. I will present results to show how it is possible to tune the electronic properties of molecular circuits within such breadboards by harnessing quantum interference phenomena and molecule-electrode couplings. Further, we will discuss an analytical/statistical method for simulating conductance histograms of complex molecular junctions, such as breadboards, which exhibit multiple conductance peaks. Using the framework, we present a strategy to experimentally test the superposition of the five embedded circuits to produce each conductance state of a bis-terpyridine based molecular breadboard.

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## Accurate and Efficient Spin–Phonon Coupling and Spin Dynamics Calculations for Molecular Solids

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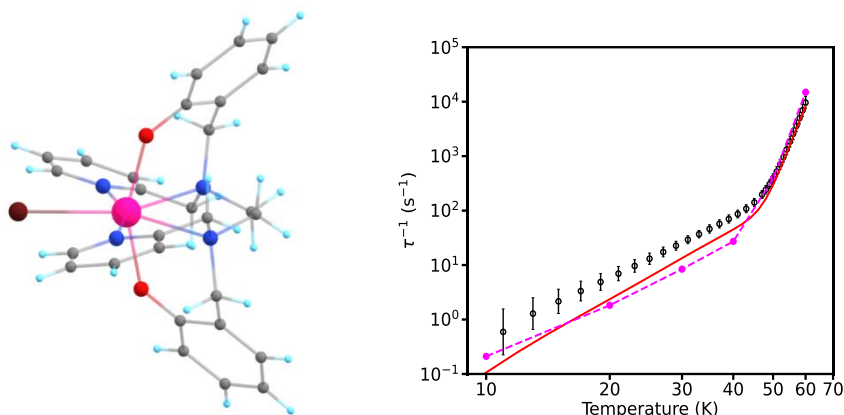
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Molecular materials are poised to play a significant role in the development of future quantum technologies. A crucial aspect of these areas is the role of spin–phonon coupling and how it facilitates energy transfer processes such as intersystem crossing, quantum decoherence, and magnetic relaxation. Here, we demonstrate the maturity of ab initio methods for calculating spin–phonon coupling by performing a case study on a single-molecule magnet and showing quantitative agreement with the experiment, allowing us to explore the underlying origins of its spin dynamics. This feat is achieved by leveraging our recent developments in analytic spin–phonon coupling calculations in conjunction with a new method for including the infinite electrostatic potential in the calculations.



**Figure 1** Molecular structure, (left) and magnetic relaxation rates (right; black exp, pink/red calc).

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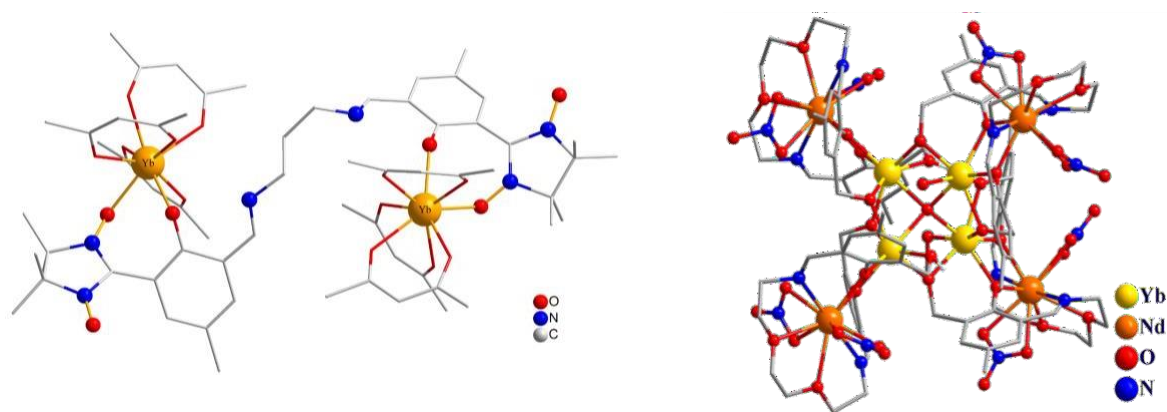
## Combined $2p/3d/4f$ chemistry: new synthetic routes towards magnetic materials

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The combination of different spin carriers ( $nd$  and  $4f$  metal ions, paramagnetic organic ligands) is a largely employed strategy for designing molecular magnetic materials. The judicious choice of ligands and metal ions allows the synthesis of a rich variety of compounds ( $2p-3d$ ,  $2p-4f$ ,  $2p-3d-4f$ ,  $nd-4f$ ,  $4f-4f'$ , etc.) with beautiful structures and exciting properties (Single Molecule Magnets, Single Chain Magnets, significant magneto-caloric effect, luminescence).<sup>1-3</sup> In this lecture I will present the main synthetic strategies towards magnetic and luminescent molecular materials, currently developed in our laboratory: (i) New polytopic nitronyl-nitroxide ligands, obtained by combining Mannich and Schiff reactions, and their complexes; (ii) Heterobi- and heterotrimetallic complexes; (iii) Coordination compounds containing two different lanthanide ions into the same molecular entity using specially designed ligands.



**Figure 1.** Left: a new family of ligands: Schiff-nitronyl-nitroxides; Right:  $4f-4f'$  heterometallic complexes constructed from heterotopic, side-off compartmental ligands.

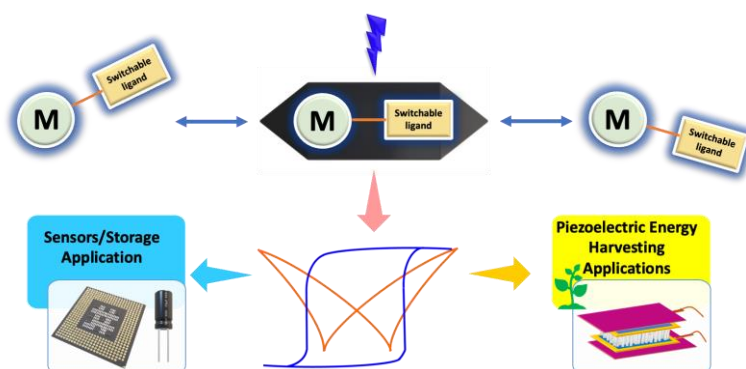
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# Molecular Ferroelectrics Derived from Switchable Metal-Ligand Coordination

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Materials that display ferro- and piezoelectric are attractive for technology applications in the area of non-volatile memory devices, electronic sensors, electro-optical systems and as piezoelectric energy harvesters, which are popularly denoted as piezoelectric nanogenerators. Small molecules with organic and hybrid organic-inorganic backbones exhibiting ferroelectric and piezoelectric properties are of major attention as alternatives for ceramic materials for their ease of synthesis and in the preparation of flexible devices based on them.<sup>1</sup> In this regard, the complex containing flexible and switchable metal-ligand coordination is attractive as it can flip under the influence of an applied electric field (Figure 1). Our group focuses on the development of ferro- and piezoelectric materials supported by phosphorus and nitrogen-centric scaffolds along with switchable metal-ligand architectures. Some recent significant results from our group in this regard are covered in this presentation.<sup>2-4</sup>



**Figure 1.** Schematic Diagram Showing the Metal-Ligand Switchable Ferroelectric Behaviour

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# Electron delocalisation and multicenter bonding in metallole-based dimeric lanthanide complexes

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The concept of sigma-aromaticity is well-known for homometallic systems mainly consisting of main group elements, with a single example involving actinides. [1,2] However, no structural reports are available on sigma-aromaticity involving heterometallic species. In this regard, we aimed to explore the concomitant  $\eta^5$  and  $\eta^1$  coordination modes of Group-14 metallole towards rare-earth elements. [3-5]

Herein, we report the synthesis, structure, electronic characterisation and computational studies of dimeric metallocene complexes based on dianionic metallole ligands  $Cp^E$  ( $E = Ge, Sn$ ) and trivalent rare-earth metals ( $M = Dy, Gd, \text{ and } Y$ ). Furthermore, we demonstrate how one-electron and two-electron reductions of the parent dimer results in significant shortening of E-E distances in the rhombic  $[M_2E_2]$  core, facilitating multicenter bonding. Structural analysis revealed increased planarity of the  $[M_2E_2]$  core upon double reduction, and enhanced electron delocalisation was observed in the electronic characterisation. [6]

NMR analysis of the mono- and doubly-reduced Y(III) complexes revealed their paramagnetic and diamagnetic nature, respectively. The addition of stoichiometric amounts of oxidising and reducing agents to the mono-reduced Y(III) dimer led to the formation of the parent dimer and doubly-reduced dimer, respectively. The reduced dimers also exhibited electron-transfer reactivity towards a variety of substrates.

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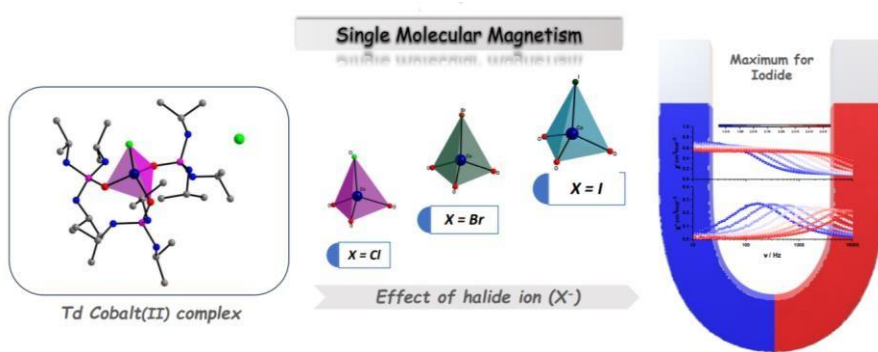
## Magnetic Behaviour of Cationic, Mononuclear, Air-stable Cobalt(II) Phosphoric Triamide Complexes

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Research in the field of magnetism has attracted attention in the past after the findings of magnetism at the molecular level. Molecules that can retain their magnetization just like bulk magnets are called single molecular magnets (SMM).<sup>1</sup> Mononuclear SMMs, known as single-ion magnets (SIMs) are also intensively investigated. These materials exhibit promising applications in high-density information storage,<sup>2</sup> molecular spintronics,<sup>3</sup> and quantum computing.<sup>4</sup> Monometallic complexes based on 3d transition metal ions exhibit appreciably enhanced magnetic anisotropy due to the stabilization of an unquenched orbital moment.<sup>5</sup> In this regard, three mononuclear tetrahedral cobalt(II) cationic complexes [Co(L)<sub>3</sub>X]X, where L = N,N',N'' tris isopropyl phosphoric triamide and X = Cl, Br, and I, have been to acquire single-ion magnetic behavior. A detailed study of the variation in the dynamic magnetic properties of the Co(II) ion in a tetrahedral ligand field has been carried out by changing the halide ligand [X = Cl (**1**), Br (**2**), I (**3**)]. Field sweep data shows the best SMM behavior for iodide complex **3** with a  $U_{eff}$  barrier of 34.9 K. The axial zero-field splitting parameter D was found to vary from  $-9.62 \text{ cm}^{-1}$  in **1** to  $-7.38 \text{ cm}^{-1}$  in **2** and  $-9.84 \text{ cm}^{-1}$  in **3**.



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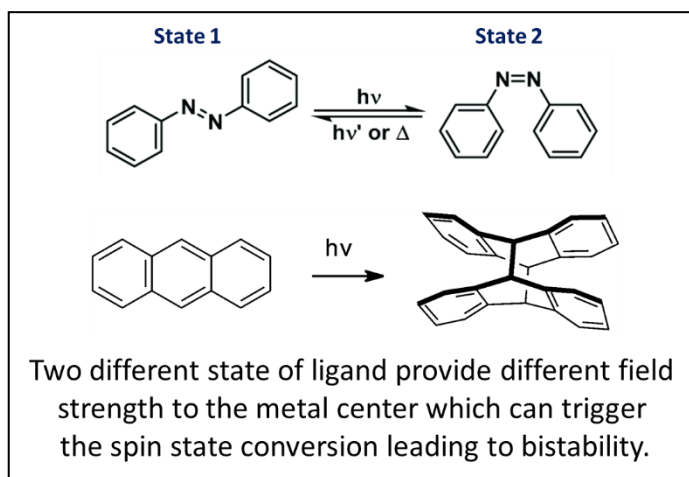
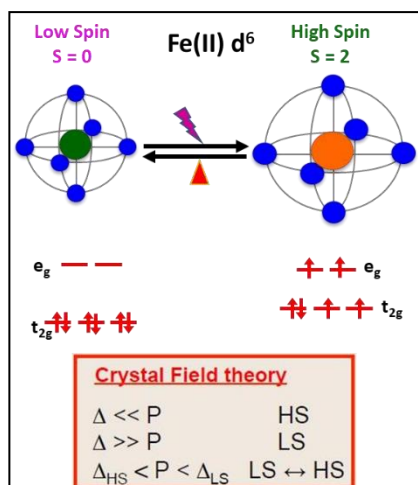
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# Modulation of Spin Crossover Behaviour *via* Photosalient Structural Transformation

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Spin crossover (SCO) is one of the most fascinating and widely studied field of research since its discovery. It has engrossed significant attention among the assorted scientific communities due to the enormous diverse applications (e.g. memory storage units, switching devices, sensors, actuators or displays *etc.*) mainly because of its molecular bistability. The bistability arises due to reversible switching between two easily accessible electronic states *i.e.* high spin (HS) and low spin (LS) with the application of external stimuli such as light, temperature, magnetic and electric field, electrochemical, chemical control *etc.* Another alternative technique to attain the bistability is selection of appropriate photoactive ligands. The ligand field-strength of such photoactive ligands can be tuned by introducing suitable light frequency. Light-induced photoisomerization of ligands can lead to corresponding *cis-trans* or ring-closing/ring-opening isomeric couples which exhibits different spin states at isothermal conditions. The present study reports the modulation of spin-crossover (SCO) behaviour *via* a photoisomerizable ligand transformation and a photochemical [4+4] cycloaddition reaction. An azo-moiety is deliberately introduced to trigger light-induced photoisomerization. On the other hand, tactical designing of ligand and suitable structural arrangements in plane brought two olefines (C=C bonds) close to each other to propagate in 1D *via* the formation of strained ring. Such dynamic photoactuating systems have potential applications in developing smart medical devices, molecular machines, artificial muscles, flexible electronics actuators, probes and microrobots.



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## Multi-technique study of the magnetic anisotropy in Co(II) Single Molecule Magnets

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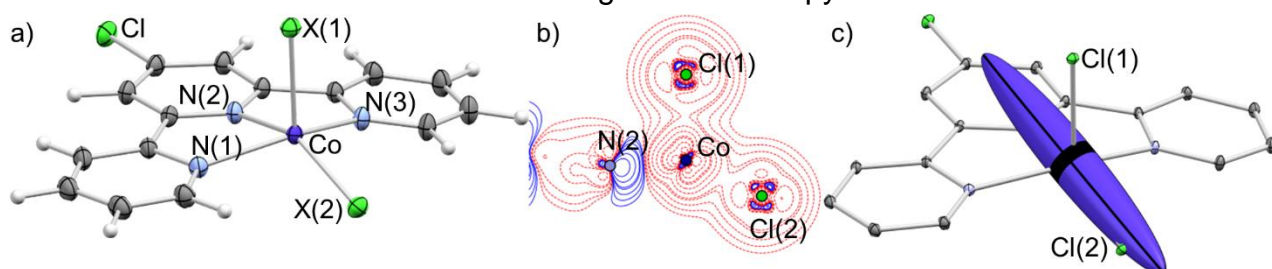
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Single-molecule magnets (SMMs) show magnetic bi-stability and slow relaxation of magnetization. For 3d-SMMs, the degeneracy and population of the d-orbitals in a specific coordination environment, determine the strength of magnetic anisotropy. Magnetic anisotropy provides SMMs with an energy barrier to magnetic reversal, hence, enhanced magnetic anisotropy implies better performing SMMs. The direction of the magnetic anisotropy can be obtained from theoretical calculations and investigated experimentally using polarized neutron diffraction and other means. From the site-susceptibility method<sup>1</sup> the susceptibility tensor for the metal atom can be derived. This technique provides unique knowledge on the magnetic anisotropy of SMMs and can be used on microcrystalline powder samples.

Here-in, two five-coordinated Co(II) complexes are investigated, [CoX<sub>2</sub>Cltpy] (X = Cl (**1**), Br (**2**). Cltpy = 4'-chloro-2,2':6',2''-terpyridine). Both **1** and **2** have distorted square-pyramidal core-geometry and easy-axis magnetic anisotropy with the calculated *D*-values, -78.87 cm<sup>-1</sup> and -60.61 cm<sup>-1</sup> respectively. The direction of the easy-axis of magnetization from *ab initio* calculation is compared against the experimentally derived easy-axis with various means such as powder polarized neutron diffraction (pPND), Multipole models of the experimental charge densities and deformation densities for **1** and **2**. From these models, the d-orbital population and detailed chemical bonding information around the Co(II) centers and the magnetic susceptibility tensor were achieved<sup>2</sup>; the results show that the experimental and theoretical direction of the magnetic anisotropy almost coincide.



**Figure 1** a) Structure of **1** and **2** (90% probability ellipsoids) {X = Cl (**1**), Br (**2**)}. b) Deformation density of **1** in the Co-Cl(1)-Cl(2) plane. c) Experimental susceptibility tensor of **1**.

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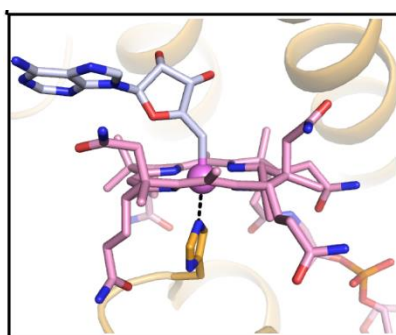
## Mechanism of Co-C Bond Cleavage in B<sub>12</sub>-Dependent Photoreceptor and the Intermediates probed by Crystallography, UV-Vis and cw-EPR/annealing Methods.

Muralidharan Shanmugam<sup>a,b</sup>, Harshwardhan Poddar<sup>a</sup>, Derren J. Heyes<sup>a</sup>, David Leys<sup>a</sup> and Nigel S. Scrutton<sup>\*a</sup>

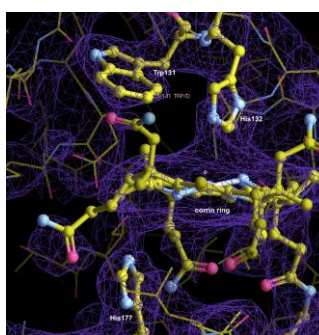
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Coenzyme B<sub>12</sub> binding proteins have gained a lot of attention recently for their ability to respond to light and act as photoreceptors.<sup>1</sup> CarH is a bacterial coenzyme B<sub>12</sub>-dependent photoreceptor involved in regulating the expression of carotenoid biosynthetic genes.<sup>1</sup> In the dark, CarH is a tetramer and suppresses transcription by binding to the promoter region. Upon illumination of CarH, the photosensitive Co-C bond in B<sub>12</sub> is cleaved, triggering a series of intermediate states which culminates in the light-adapted, monomer formation and release of DNA. The nature of the Co-C bond cleavage (homolytic vs heterolytic), roles of the amino-acids surrounding the active-site/excess molecular oxygen and the different intermediates formed during the photocycle are poorly understood.<sup>2-4</sup>



dark-adapted state



photoactivated state

In this presentation, the crystal structures of the native and photo-activated CarH from *Thermus thermophilus*, TtCBD enzyme and the associated dynamics of the B<sub>12</sub>-chromophore during the photocatalysis will be discussed.<sup>5</sup> The cryo-trapping experiment at various temperatures along with cw-EPR/annealing and spin-trapping techniques revealing the possible intermediates present along the CarH photocycle. The role of the axial H132 ligand, and excess molecular oxygen in the photocycle and the UV-Vis data of these enzymes will also be discussed in detail.

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# Masked Divalent Reactivity of Heterobimetallic Lanthanide Isocarbonyl Complexes

Arpan Mondal,<sup>a</sup> Jinkui Tang,<sup>b</sup> Richard Layfield<sup>\*a</sup>

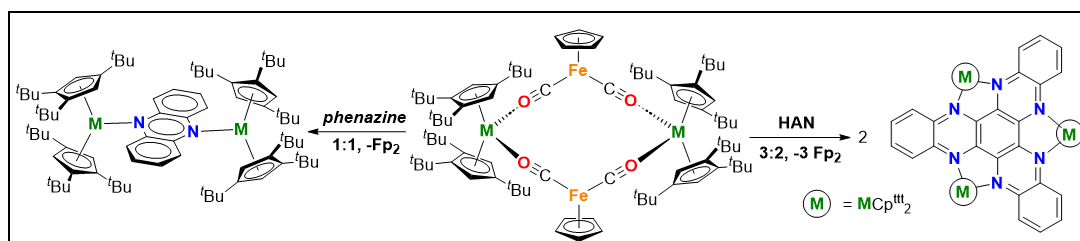
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Recently, divalent lanthanide metallocenes have attracted significant attention due to their small molecule activation chemistry and single-molecule magnet (SMM) behaviour.<sup>1,2</sup> Metallocenes of the 'non-classical' divalent lanthanides (Dy, Tb, Ho, Nd, Er) are of great interest here as they can form radical-bridged complexes in reactions with N-heterocycles, leading to SMMs with strong magnetic hysteresis with coercivity, and high blocking temperatures ( $T_B$ ).<sup>3,4</sup> However, isolation of non-classical divalent lanthanide metallocenes is challenging as they are highly reactive and often only stable at low temperatures.

To circumvent this problem, we have considered that the cyclopentadienyliron dicarbonyl anion ( $Fp^-$ ) can behave as a reducing agent, readily losing an electron to form  $Fp_2$ . We reasoned that the  $Fp^-$ -bridged lanthanide metallocene  $[(Cp^{ttt})_2Ln\{-m-(OC)_2FeCp\}]_2$  ( $Ln = Dy^{III}, Y^{III}$ , and  $Cp^{ttt} = 1,2,4$ -tri-tert-butylcyclopentadienyl) would also behave as reducing agents and, therefore, could be surrogates for divalent lanthanides. The target compounds were synthesized according to Scheme 1.



**Scheme 1.** Reactivity of  $Fp^-$  anion bridged lanthanide metallocenes.

The magnetic study reveals the presence of slow relaxation of magnetization under zero field for the  $Fp^-$ -bridged dysprosium complex, which is also confirmed by ab initio investigations. Further, it has been observed that these complexes can easily eliminate  $Fp_2$  dimer and reduce N-heterocyclic compounds, to give radical bridged trimetallic SMMs (Scheme 1).

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# Room Temperature Giant Magnetolectric Coupling for Magnetic Energy Harvesting in Single Phase $\{Co^{III}_3Dy^{III}\}$ Molecular Nanogenerator

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Revealing single-phase multiferroic (MF) materials in conventional bulk oxides is an exceptionally daunting task. However, achieving strong magnetolectric (ME) coupling at room temperature (RT) in these materials is even more formidable despite their envisioned applications in multi-state memory storage devices, spintronics, magnetic field sensors, etc. The weak ME coupling in single-phase MF materials is primarily due to the ferro/antiferromagnetic ordering observed at very low temperatures, contrasting with ferroelectric ordering typically discerned at RT. These challenges can be effectively addressed by leveraging discrete molecular-based MF materials. Nonetheless, molecular-based ferroelectric materials remain in their infancy due to challenges in achieving polar point groups in these complexes. By overcoming these hurdles through meticulous molecular engineering, we have unveiled a discrete molecular complex,  $[Co^{III}_3Dy^{III}(L)_6] \cdot 4MeOH$  ( $Co_3Dy$ ), which exhibits an unprecedentedly strong ME coupling constant ( $\alpha$ ) value of  $250 \text{ mVcm}^{-1}Oe^{-1}$  at RT. This robust ME coupling at or above RT presumably originates from the coupling between magnetostriction and ferroelectric phenomena observed in the paramagnetic  $Co_3Dy$  complex. To demonstrate the ME coupling and harness the large  $\alpha$  value, we have developed an ME nanogenerator device using  $Co_3Dy$  to convert weak stray magnetic fields into electrical energy. This device produces an output voltage of  $\sim 430 \text{ mV}$  and an output current of  $0.3 \mu A$  under a small AC magnetic field amplitude of  $24.2 \text{ Oe}$ .

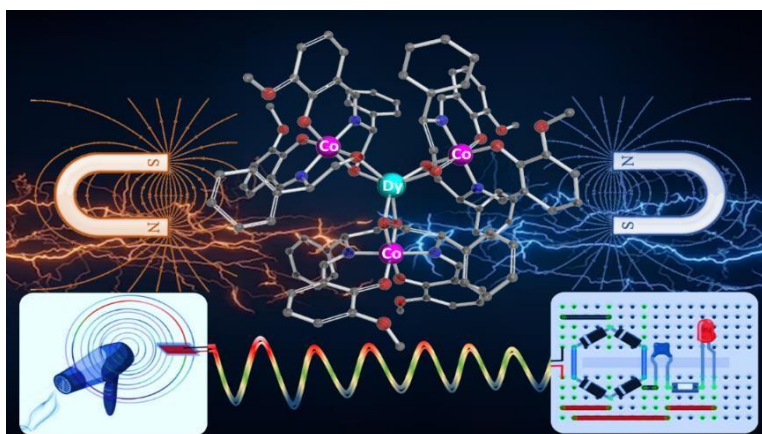


Fig: Schematic representation of the  $\{Co_3Dy\}$  complex exhibiting effective magnetolectric coupling for energy harvesting.

## From Ultrafast Photoinduced Small Polarons to Cooperative and Macroscopic Charge-Transfer Phase Transition

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R. Bertoni,<sup>a,b</sup> M. Lorenc,<sup>a,b</sup> Celine Mariette,<sup>d</sup> Marco Cammarata,<sup>d</sup> Matteo Levantino,<sup>d</sup>  
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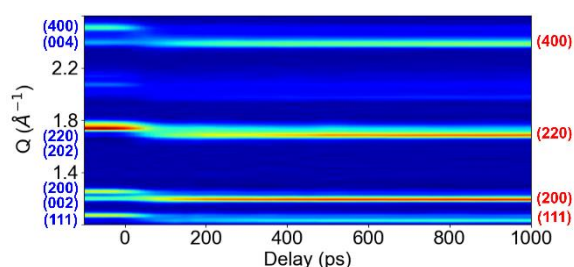
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Ultrafast photoinduced phase transitions (PIPT) at room temperature, driven by a single laser shot and persisting long after stimuli, represent emerging routes for ultrafast control over materials' properties. Time-resolved studies of such far from equilibrium dynamics, driving crystalline solids through collective transformations into new phases, provides fundamental mechanistic insight into electronic and structural transformations, for optimizing materials' photo-response. Here we study PIPT for a  $\text{RbMn}[\text{Fe}(\text{CN})_6]$  material, exhibiting a 75 K wide thermal hysteresis centered at room temperature between a  $\text{Mn}^{\text{III}}\text{Fe}^{\text{II}}$  tetragonal phase and a  $\text{Mn}^{\text{II}}\text{Fe}^{\text{III}}$  cubic phase. We used a sample streaming technique to monitor the out-of-equilibrium dynamics by ultrafast X-ray diffraction and X-ray or IR spectroscopies, for tracking atomic and lattice reorganizations and symmetry changes.<sup>1,2,3</sup> At low laser fluence, photoinduced charge-transfer polarons form within 200 fs, which are responsible for lattice distortion and expansion. Above threshold fluence, the PIPT occurs within 10's ps towards the permanent  $\text{Mn}^{\text{II}}\text{Fe}^{\text{III}}$  cubic state.



**Figure 1.** Time-resolved XRD pattern of  $\text{RbMn}[\text{Fe}(\text{CN})_6]$ . The PIPT is characterized by the merging of the tetragonal (200) and (002) Bragg peaks into a single (200) cubic peak.

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# Unveiling Solid State Luminescence from Ultra-thin Noncovalent Two-dimensional Molecular Crystals Fabricated at Air-Water Interface

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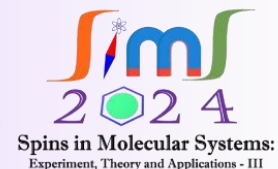
Two-dimensional (2D) molecular crystals represent an important class of materials for advanced optoelectronic applications. Owing to the monolayer or few-layered thickness, unique properties can be realized from the 2D molecular crystals which are different from the bulk organic counterparts. We introduce a promising pressure-triggered strategy to fabricate noncovalent free-standing 2D molecular crystals (1, 2). The molecular thick, micron long, yet stable 2D molecular crystals are formed in a controllable and efficient way on the flat-water surface having small roughness. Formation of 2D molecular crystals at different stages is monitored using in-situ synchrotron grazing incidence X-ray diffraction measurements and atomic force microscopy. The crystal structures are probed using in-situ synchrotron grazing incidence X-ray diffraction measurements and selected area electron diffraction pattern using transmission electron microscopy. Resultant 2D molecular crystals show a marked enhancement of luminescence in the solid state. The critical conformation of molecules within the 2D crystals concomitantly leads to the reduced singlet-triplet energy gap and strong spin-orbit coupling for effective mixing of the singlet and triplet states, which explains the room temperature phosphorescence origin of the luminescence and luminescence enhancement.

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## Spin Evolution in Molecular Structures

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Spin evolution in molecular structures is pivotal in processes like singlet fission, which is particularly relevant in organic photovoltaics and photonics. In singlet fission, a single excited singlet state can split into two triplet states, a phenomenon commonly observed in organic materials. This multiexciton generation holds the potential to exceed the Shockley–Queisser limit for photovoltaic devices, enhancing their efficiency.

The fission process is influenced by the electronic structure of the materials and the presence of specific substituents. Molecules exhibiting strong coupling between singlet and triplet states are more likely to demonstrate efficient singlet fission.

The interplay between spin evolution in molecular structures and the mechanisms of singlet fission represents an exciting area of research with significant implications for advancing energy conversion technologies. In this talk, I will discuss molecular design and synthesis strategies aimed at optimizing exchange energy and morphology, critical factors for facilitating singlet fission in suitable materials.

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## Meticulous extraction of the multispin Hamiltonian in dicobalt(II) complexes out of *ab initio* calculations

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In the field of computational molecular magnetism, it is common practice to focus on single-ion anisotropies and isotropic couplings. Extracting anisotropic exchange terms requires demanding calculations and also more complex analyses. In calculations based on quasi-relativistic and multiconfigurational wavefunction approaches for molecular magnets, an extensive set of many-electron states is typically computed in the presence of the spin-orbit coupling. Refocusing on a model space of a smaller subset of energy levels involves applying effective Hamiltonian theory.<sup>1</sup> The size of this “model” space quickly grows with the local spins and the number of active magnetic centers.

In this presentation, I will showcase a specific strategy that successfully extracts anisotropy parameters and coupling constants in dicobalt(II) complexes in the weak-exchange limit.<sup>2</sup> With two high-spin cobalt(II) magnetic centers (local quartets), the model space for the binuclear complexes includes 16 spin functions, assuming orbital degeneracy is not a factor. Two case systems will be studied, and a previous dinickel(II) complex will be revisited.

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## Electric polarization control via electron transfer

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The development of novel molecular compounds, whose physical properties can be controlled by external stimuli, have attracted considerable attention. We have synthesized several polar compounds, in which the electric polarization can be switched via thermal- and photo-induced electron transfer or spin transition process.<sup>1-4</sup> A typical example is the [CoGa] heterometallic dinuclear complexes.<sup>1</sup> The [CoGa] complex exhibits thermally-induced electron transfer between the metal and ligands,  $\text{Co}^{\text{III-LS}}\text{-d}^{\text{h}^3}\text{bq}^3\text{-Ga}^{\text{III}} \rightleftharpoons \text{Co}^{\text{II-HS}}\text{-d}^{\text{h}^2}\text{bq}^2\text{-Ga}^{\text{III}}$ , which involves changes in the molecule's dipole moment. Since the [CoGa] complexes are designed to be oriented in the same direction within the crystal via chiral ligands, intramolecular electron transfer causes the polarization to switch at the crystal level. This polarization switching is also induced by incident photons. Another example is the [FeCo] heterometallic dinuclear complexes.<sup>2</sup> The [FeCo] dinuclear complex exhibits a magnetic field-induced spin crossover process, resulting in a significant polarization change. Furthermore, molecular cyanide-bridged [FeCo] bimetallic Prussian blue analogues switches the system between the electron-transferred metastable state and the ground state. We successfully executed a nonpolar-to-polar phase transition in a trinuclear cyanide-bridged [Fe<sub>2</sub>Co] complex crystal via directional electron transfer.<sup>3</sup>

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## Quantum Control of Molecular Carbon

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Magnetic states in graphene nanostructures have undergone intense theoretical scrutiny, because their coherent manipulation would be a milestone for spintronic and quantum computing devices. In nanoribbons, experimental investigations now show that quantum coherence of edge and localized graphene states is observable.[1] Several questions remain thus unsolved: how can molecular spins be integrated into electronic structures? Can topological states be used to improve the quantum coherence? Can metals be introduced so as to affect the carbon spin states? Can the quantum spin states be observed in devices? What is the role of electron-electron correlations? Here we try to provide an answer to these questions, exploring spin states in carbon by using molecular synthetic techniques.

Here we show how topological engineering of the carbon lattice can lead to improved coherence, higher than theoretical predictions.[2,3] We then show how such molecular structures can be included into molecular devices, producing magnetoresistive effects that are opposite to non-molecular devices.[4,5,6] The inclusion of metals then allows altering the spintronic properties. [7] We show how such electronic devices show quantum blockade up to room temperature, with different Luttinger liquid regimes available in different ranges.[8] The bright emissive modes offer the possibility of observing the quantum states optically.[9]

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## Controlling Hall response in epitaxial $Mn_3Sn$ thin films

Shouvik Chatterjee

Non-collinear antiferromagnet  $Mn_3Sn$  has been shown to exhibit large anomalous Hall effect at room temperature and is a promising material system for spintronics applications<sup>1-5</sup>. However, so far anomalous Hall effect has only been observed with magnetic field lying within the Kagome plane. In this talk, I will show how anisotropic strain along with in-plane Dzyaloshinskii-Moria interaction arising from broken inversion symmetry at the heterointerfaces can imprint finite scalar spin chirality in Kagome lattices such as  $Mn_3Sn$ . The finite canting of the Mn spins out of the Kagome plane breaks both mirror and time-reversal symmetries that allows non-zero anomalous Hall conductivity with magnetic field applied perpendicular to the Kagome plane, which we observe in our epitaxial thin films. We also observe the appearance of topological Hall like signatures at lower temperatures, the stability of which can be controlled by varying the thickness of these thin films. I will show evidence for heat assisted switching of the anomalous Hall effect at room temperature and of the topological Hall like features by the application of electric pulse with modest current densities of  $\sim 1.8 \times 10^{10}$  A/m<sup>2</sup>. This allows us to access multiple-stable, non-volatile anomalous Hall resistance memory states, which could be attractive for spintronics and neuromorphic computing schemes. Our results establish the potential of realizing novel functionalities in  $Mn_3Sn$  by thin film engineering.

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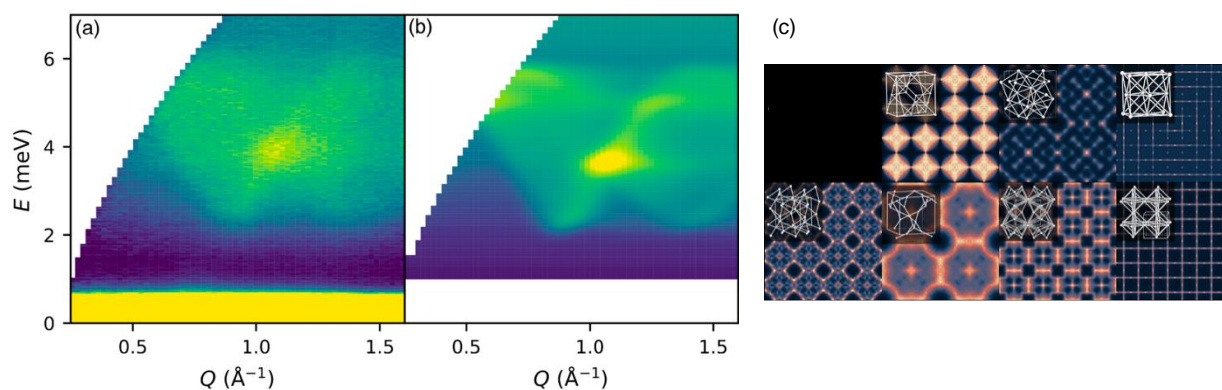
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## Modular metal-organic materials towards unconventional function

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Metal-organic magnets offer unique opportunities for control over magnetic function, as chemical functionalisation of the framework structure allows for tuning of the functional behaviour while retaining the structural and hence magnetic topology. In this talk I will highlight how this can be used to realise collective magnetic properties challenging to realise in classical dense inorganic materials. I will highlight experimental work on the family of layered metal organic magnets  $MCl_2(L)$  comprising metal halide chains connected by a molecular ligand (pyrimidine, 2,1,3-benzothiadiazole). This platform allows us to realise a range of different properties, from routes towards the Haldane  $S=2$  quantum chain<sup>1</sup> to controllable non-collinear ferromagnetism.<sup>2</sup> I will also show how the diversity of high symmetry topologies realisable in metal-organic frameworks offers opportunities to produce new spin liquid phases.<sup>3</sup> I will also show how neutron scattering can be invaluable for metal-organic magnets, provide otherwise challenging to obtain insights into both the ground states, from Bragg scattering, and interactions of magnetic materials, from modelling of magnetic diffuse scattering and powder inelastic scattering.



**Figure 1** Inelastic powder neutron spectrum of  $CrCl_2(\text{pyrimidine})$  (a) experimental and (b) linear spin wave calculations. (c) predicted diffuse scattering for the predicted classical spin liquid

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## Tailoring Spin Textures in Non-centrosymmetric 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 spintronics application. We show a class of polar non-centrosymmetric ferroelectric systems have all the necessary ingredients to host Rashba-Dresselhaus effect. We shall argue in addition to crystal symmetry, the orbital character of the bands at a particular k-point and the associated symmetry plays a crucial role in stabilizing persistent spin texture (PST) that maintain a uniform spin-configuration in the momentum space in these systems[1,2]. We show a class of non-polar half-Heusler alloys with rich local symmetry of the wavevectors display Dresselhaus effect, Rashba effect with both linear and non-linear terms, non-trivial Zeeman spin splitting and band splitting with vanishing spin polarization making them ideal candidate for application in spin valleytronics. Finally we show the realization of persistent spin textures in non-polar chiral systems [4].

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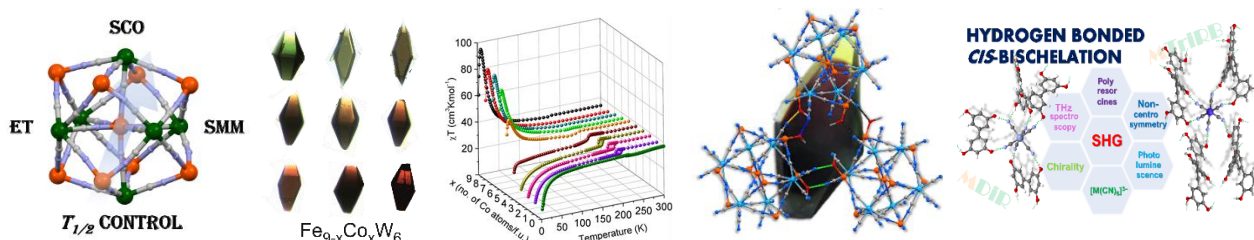
## Spins in multicomponent cyanidometallate-based systems: selective spin state switching and optical properties

R. Podgajny\*<sup>a</sup> and all coauthors of articles cited as refs. 1, 2, and 4

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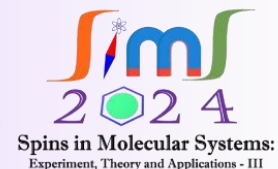
Polycyanidometallate-based systems offer attractive platforms for functionality exploiting specific structural features, structural non-rigidity, and related physicochemical properties. In this context, we present speciation of coordination sites and tuning of magnetic exchange coupling, electron transfer (ET), and spin-crossover (SCO) properties in  $[M(CN)_8]^{3-}$  bi- 3d-5d and trimetallic 3d-3d'-5d or 3d-5d-5d' cyanido-bridged clusters,<sup>1</sup> as well as in the related multiphase molecular crystal@crystal composites.<sup>2</sup> Next, considering the recent reports on tuning of spin state switching in the related co-crystalline phases,<sup>3</sup> we present new  $\{[M(CN)_6]^{3-}; \text{oligoresorcinol}\}$  ( $M = \text{Cr, Fe, Co}$ ) based co-crystal salts disclosing cyclic  $\{C_6H_4-(O-H \cdots NC)_2M(CN)_4\}$  hydrogen-bonded synthons, local chirality, and lattice non-centrosymmetry, to produce second harmonic generation (SHG) and tunable photoluminescence (PL). Our results will be discussed in terms of to-be-realized more advanced architectures and their functional performance.



**Figure 1** Highlights of the  $[M(CN)_x]^{n-}$  based multicomponent systems of interest in Multicomponent Hierarchical Molecular Architectures (WHAM) group, Faculty of Chemistry, JU in Krakow.

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## Electronic Structures of High-Valent Metal Complexes with Diverse Spin States

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High-valent metal ions strapped with macrocyclic ligands are potent catalysts enabling small molecule activation. [1] Heme and non-heme enzymes form high-valent 3d-metal ions as active intermediates. [2] Electronic structure calculations of high-valent metal ions bound to synthetic receptors behave uniquely to those of enzyme analogues. We propose supramolecular hosts as ligands that can enable regioselective oxidation of alkanes. We will highlight using high-valent vanadium and iron oxygen adducts strapped to a cucurbituril host to catalyze unactivated alkanes at room temperatures. We have also used a cobalt catalyst that can enable water oxidation. The spin states of these transition metal supramolecular catalysts are vastly different to those of several existing synthetic mimics. The role of the host is not just the ligand but it takes parts in the reactivity as secondary interactions with the substrates.

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## From Spin Materials to Electron Transfer Catalysis

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The major concerns about industrially used catalytic systems today are: i) the high cost of catalysts; ii) the toxicity of heavy transition metals; iii) difficulties in removing trace amounts of toxic-metal residues from the desired product; and, finally, iv) rare transition metal depletion, which does not meet the requirement of sustainable development. Developing environmentally friendly catalysts is an excellent option in this regard. Naturally, the most recent trend in catalyst development heralded a new era of metal-free catalysis or catalysts based on earth-abundant, nontoxic, and low-cost metals. This talk will review our recent advances in using small organic molecules to mimic transition metal-based catalysis systematically. We designed electron transfer catalysis using the smallest polycyclic odd alternant hydrocarbon, phenalenyl (PLY)-based molecules, inspired by a completely different field of molecular spin materials. This talk will focus on how to avoid transition metals when performing various cross-coupling catalysis.



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## How to create giant anisotropic interactions in poly-nuclear magnetic systems and impact of the electric field on anisotropic interactions: New insights from theory

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Magnetic anisotropy is the origin of the single molecule magnet (SMM) behavior which consists of a slow relaxation of the magnetization and a blocking of the magnetization for sufficiently low temperatures. This behavior can lead to technological applications in the field of quantum computing and also arouses the interest of researchers in the fundamental area of quantum mechanics. Thanks to collaborative theory/experiment works, the nature and magnitude of the microscopic interactions at work in mononuclear complexes are now relatively well mastered. Nevertheless, the anisotropic interactions between several magnetic centers within poly-nuclear compounds are still very poorly understood. Furthermore, the control of magnetic properties by means of an external perturbation is also a crucial issue if we one-day wish to use these systems in devices for application purposes. These subjects are the objects of the work presented here. We will see how first order spin-orbit couplings can considerably increase the local anisotropies of magnetic centers, their anisotropic exchange coupling and the Dzyaloshinski Moriya interaction.<sup>1,2</sup> Finally, we will focus on the impact of the electric field<sup>3,4</sup> (perturbation likely to make the control of magnetic properties possible) affects all these different interactions.

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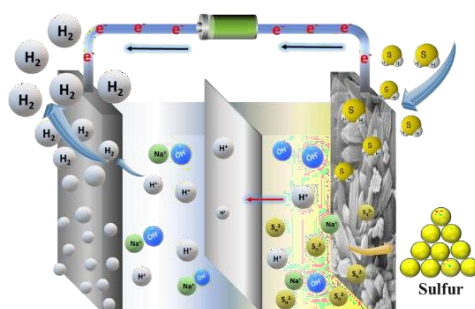
## Designing greener energy conversion system for a sustainable future

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Highly efficient and cost-effective hydrogen production ( $H_2$ ) promises to play a vital role in green energy production due to its high energy density, low-pollution, and renewable nature. The electrocatalytic decomposition of  $H_2O$  to  $H_2$  and  $O_2$  considered to be the most sustainable method for pure  $H_2$  production, unfortunately, it stumbles due to potentially uphill and energy-consuming sluggish anodic oxygen evolution reaction (OER).<sup>1</sup> Contrary to  $H_2O$  isostructural hydrogen sulfide ( $H_2S$ ) possesses lower bond dissociation energy. Therefore, anodic sulfide oxidation reaction (SOR) will be more energy-efficient than OER. Presently, the Claus process is the most popular industrial technology for removing  $H_2S$ , but energy wasted in the form of steam. Therefore, electrochemical conversion of environment pollutant  $H_2S$  into  $H_2$  and S provide a way to remove pollutant  $H_2S$  and also emerges as new energy source.<sup>2</sup> However, the industrialization of such energy-efficient technology never meets the expectation in reality in the absence of cost-effective and robust electrocatalyst. My talk addresses the approach towards  $H_2S$  electrocatalysis and noble-metal free based catalyst that exhibited lower onset potential of 0.23 V vs. RHE towards SOR, which is 1.25 V lower than OER. Notably, only a 1.2 V commercial battery easily derives  $H_2S$  electrolysis, which is impossible for  $H_2O$  splitting demonstrating the tremendous future prospective of  $H_2S$  for cost effective hydrogen production as well as sulfur which can be utilized as a cathode/anode catalyst for sulfur based battery for a sustainable economy.<sup>3,4</sup>



**Scheme 1.** Schematic representation of  $H_2S$  electrolysis into cathodic  $H_2$  and anodic SOR.

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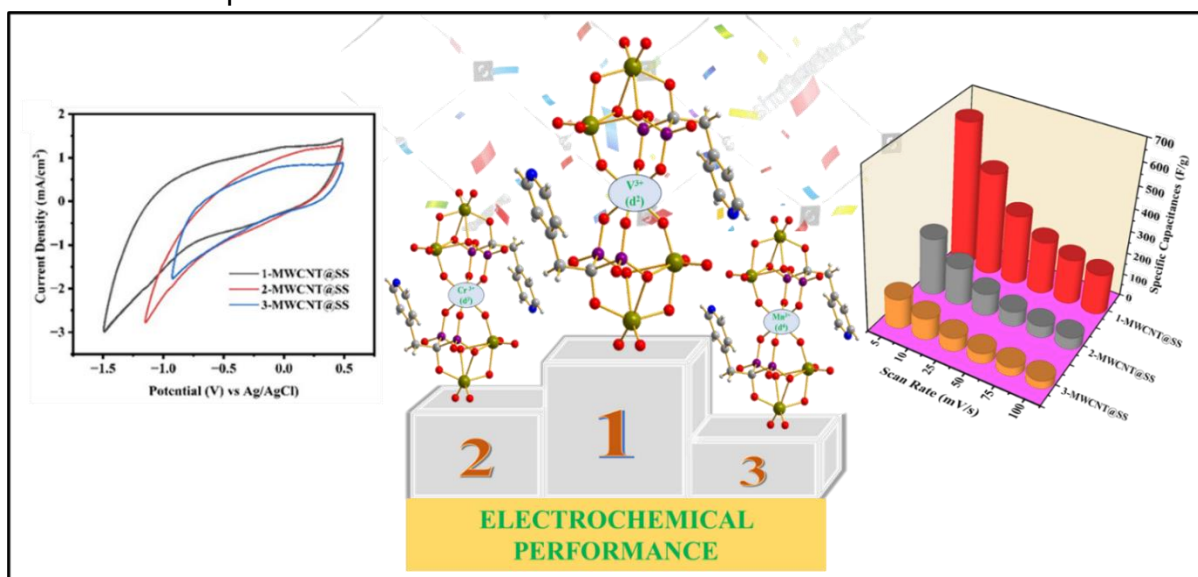
# Investigations into the Electrochemical Energy Storage Properties of Diphosphonate derivatives of Oxo-vanadates: Experiment and Theory

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**Abstract:** Electrochemical supercapacitors have become popular and pivotal as energy-storing devices; having immense potential along with remarkable properties, like excellent fast charging capacity, high power density, and long-lasting cyclic stability. Vanadates, with their unique redox and coordination properties, have also found important applications energy storage. Oxo-vanadates with diphosphonate ligands, are a relatively newer class of materials. Such ligands are observed to stabilize multiple oxidation-states of the metal in the same complex, making them extremely versatile electrochemically. From our studies with mixed-metal molybdate complexes,  $[(\text{Mo}^{\text{VI}}_2\text{O}_5)_2(\text{MO}_2)\{\text{O}_3\text{P}-\text{C}(\text{O})(\text{CH}_2-4-\text{C}_5\text{NH}_4)-\text{PO}_3\}_2]^{7-}$  [where  $\text{M} = \text{V}(\text{III}), \text{Cr}(\text{III}), \text{Mn}(\text{III})$ ], we have observed highest efficiency with the molybdenum-vanadium systems, exemplifying the better redox activity of vanadium. Our subsequent studies with mixed-valent vanadates  $[(\text{V}^{\text{IV}}\text{O}_2)(\text{V}^{\text{V}}_2\text{O}_5)_2\{\text{O}_3\text{P}-\text{C}(\text{O})(\text{CH}_2-n-\text{C}_5\text{NH}_4)-\text{PO}_3\}_2]^{10-}$  ( $n = 2, 3$ ), and shows greater electrochemical efficiency with respect to the mono-valent vanadate complex  $[(\text{V}^{\text{IV}}\text{O})_3(\text{O})\{\text{O}_3\text{P}-\text{C}(\text{OH})(\text{CH}_2-4-\text{C}_5\text{NH}_4)-\text{PO}_3\}_3]^{8-}$ . Furthermore, presence of encapsulated guest molecules within the capsular assemblies of the complexes  $[(\text{V}^{\text{V}}\text{O})_2(\text{V}^{\text{IV}}_4\text{O}_8)_2\{\text{O}_3\text{P}-\text{C}_6\text{H}_4-\text{PO}_3\}_4] \cdot 2\text{H}_2\text{O}]^{10-}$  and  $[(\text{V}^{\text{V}}\text{O})_2(\text{V}^{\text{IV}}_4\text{O}_8)_2\{\text{O}_3\text{P}-\text{C}_6\text{H}_4-\text{C}_6\text{H}_4-\text{PO}_3\}_4] \cdot 2\text{DMF}]^{10-}$  creates significant differences in their electrochemical performances.



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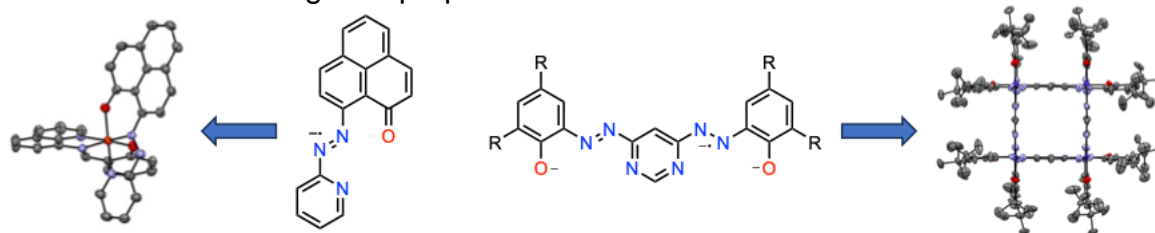
## Exploring single-component spin-crossover conductors using redox-active ligands

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We have a long-standing interest in the use of spin-bearing radical ligands to add electronic functionality to coordination complexes, including within molecular switches such as spin-crossover complexes and valence tautomers<sup>1,2</sup>. This requires the synthesis of pi-extended redox-active ligands where multiple oxidation states can be addressed through metal/ligand electron transfer processes. Substituted diarylazo ligands can be readily prepared and have desirable redox properties in this regard<sup>3,4</sup>. In this presentation we will discuss several of these ligands and their coordination complexes (Fig. 1) with typical “spin-crossover” transition metals ions ( $\text{Fe}^{2+/3+}$ ,  $\text{Co}^{2+}$ ,  $\text{Mn}^{3+}$ ). We have observed complexes featuring ligand mixed-valency, very narrow HOMO-LUMO gaps and open-shell ligand character, which results in electrical conductivity. Our goal is to couple the temperature and/or light induced spin state change to electrical conductivity properties to produce new single-component conductors with switchable magnetic properties.



**Figure 1** Selected redox-active ligands and complexes to be discussed

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## Chirality Induced Spin Selectivity (CISS) effect with helicene and tetrathiafulvalene derivatives

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A sustainable future requires highly efficient energy conversion and storage processes, where electrocatalysis plays a crucial role. The activity of an electrocatalyst is governed by the binding energy towards the reaction intermediates, while the scaling relationships prevent the improvement of a catalytic system over its volcano-plot limits. To overcome these limitations, unconventional methods that are not fully determined by the surface binding energy can be helpful. In this respect, thiadiazole-[7]helicene and bis(thiadiazole)-[8]helicene have been used to boost the oxygen evolution reaction (OER) by up to ca. 130 % (at the potential of 1.65 V vs. RHE) at state-of-the-art 2D Ni- and NiFe-based catalysts *via* the CISS effect.<sup>1</sup> Our results show that the chirality of the helicene molecules is accountable for the great enhancement in the activity of state-of-the-art OER catalysts through the so-called chirality induced spin selectivity (CISS) phenomenon.<sup>2</sup> The comparison of different electrode configurations provides a clear guideline for optimizing the enhancement.<sup>3</sup> In this contribution we will discuss as well evidences for the occurrence of the CISS effect in chiral tetrathiafulvalenes (TTF)<sup>4</sup> and in [6]helicene-bis(thiol) through single molecule break junction.<sup>5</sup> In the latter, the concomitant observation of the CISS and the electrical magnetochiral anisotropy (eMChA) effects was possible.



Figure 1 CISS versus eMChA in chiral materials

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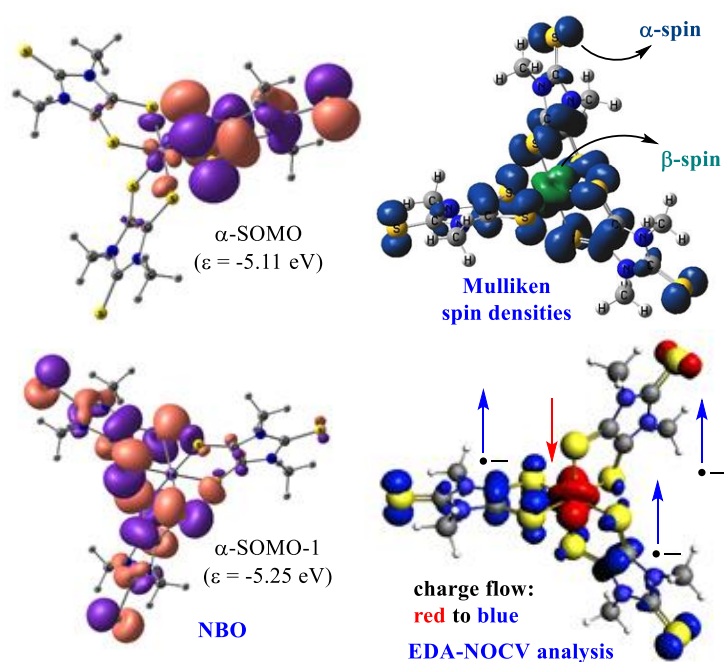
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## Electronic Structures of Stable Metal-Radical Complexes

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Enzyme plays pivotal roles in biological systems for existence of life. Most of the metallo-proteins contain metal-complexes, called cofactor, each of which has chemical roles to play via elementary chemical or electrochemical processes in a specific coordination environment. The coordinating atoms of those co-factors are partially or entirely sulfur atoms which control the redox activities and chemical processes of metal centres or coordination metal clusters. Thiolene is a class of two sulfur -donor ligands, which is redox non-innocent in nature ranging is charge from zero to di-negative (neutral singlet, anionic doublet and di-anionic singlet). Thiolene unit is also part of Mo-containing protein (pyranopterin cofactor). In addition, many co-factors of enzymes possess M-S bonds. Very recently air and moisture sensitive redox non-innocent N-heterocyclic carbene (NHC) functionalized (C2, C4, C5) tri-sulfur compound which behaves as a thiolene ligand  $[(SS-NHC=S)^0 \rightarrow (SS-NHC=S)^{\bullet-} \rightarrow (SS-NHC=S)^{2-}]$  isolated by Robinson et al.<sup>1</sup> Herein, I will present synthesis, isolation, characterization (UV-vis-NIR, XPS, CV, EPR and magnetic properties) and electronic structure of metal-radical complexes of two sulfur donor radical anion ligand  $[(SS-NHC=S)^{\bullet-}]$ .



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**MODERN TRENDS IN MOLECULAR MAGNETISM – IV**  
**&**  
**SPINS IN MOLECULAR SYSTEMS:**  
**EXPERIMENT, THEORY AND APPLICATIONS – III**



**Michael Shatruk**



**Organized by Team M2S**

## Spin triangles: from magnetoelectric couplings to spin-electric transitions

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Electric fields represent an ideal means for controlling spins at the nanoscale and, more specifically, for manipulating protected degrees of freedom in multispin systems.<sup>1,2</sup> In previous work, the required magnetoelectric coupling for such manipulations, was demonstrated within the ferric complex  $[\text{Fe}_3\text{O}(\text{O}_2\text{CPh})_6(\text{py})_3]\text{ClO}_4 \cdot \text{py}$  ( $\text{Fe}_3$ ) using Electron Paramagnetic Resonance under electric fields.<sup>3,4</sup> Recently, low-temperature magnetic far-IR spectroscopy on  $\text{Fe}_3$  provided the first experimental evidence of spin-electric transitions in polynuclear complexes, allowing us to estimate the spin-electric coupling.

In this lecture, the basic attributes of spin triangles as a class of molecules will be presented as well as their perspectives as electrically controlled magnetic nano-objects.

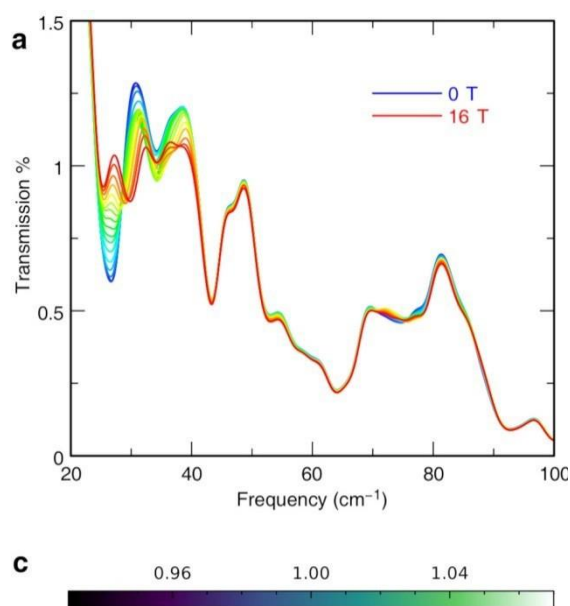


Figure. Variable-field magneto-FIR spectra of  $\text{Fe}_3$ .

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## High sensitivity magnetometry with quantum defects in diamond

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Nitrogen-vacancy (NV) defect centers are versatile quantum sensors which are able to measure a number of physical quantities such as magnetic field, electric field, temperature and stress/strain at ambient conditions [1-4]. After introducing the unique optical and spin properties of NV centers, we discuss our current research efforts on ODMR-based high sensitivity magnetometry using ensembles of NV centers in diamond lattice.

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## Probing Spin Polarized Electron Dynamics in Yttrium Iron Garnet Using Circularly Polarized XUV Light

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This talk describes the recent ability to directly observe spin-polarized electron dynamics at semiconductor surfaces using XUV Magnetic Circular Dichroism (XUV-MCD). The ability to produce spin polarized currents at interfaces underlies many applications ranging from information processing to enantioselective photocatalysis; however, designing materials to support these applications requires an improved understanding of spin-dependent electron dynamics at interfaces. Towards this goal, XUV-MCD reflection-absorption spectroscopy provides direct observation of spin dynamics with ultrafast time resolution and surface sensitivity. Using this technique, we perform a detailed spectroscopic investigation of the spin dependent electron dynamics in yttrium iron garnet ( $Y_3Fe_5O_{12}$ , YIG) that give rise to efficient, spin selective photocatalysis.<sup>1</sup>

YIG is a ferrimagnetic oxide with a visible band gap, consisting of two sub-lattices based on octahedrally and tetrahedrally coordinated Fe(III) centers. Ultrafast measurements using linearly polarized XUV light show a 70% reduction in the formation of surface electron polarons in YIG compared to hematite due to site-dependent electron-phonon coupling. Circularly polarized XUV-MCD measurements show that spin-aligned holes accumulate in the hybridized O  $2p$  / Fe  $3d$  valence band giving rise to spin-polarized Fe(IV) redox-active states in the octahedral sublattice of YIG. These long-lived, spin aligned holes improve the selectivity of water oxidation to  $O_2$  by favoring the triplet reaction pathway over the single pathway to produce  $H_2O_2$ . Together, these results provide a detailed understanding of enhanced water splitting efficiency using a spin-selective photocatalyst and open the door for probing the effects of spin-polarized currents in systems ranging from magnetic oxides to chiral matter.

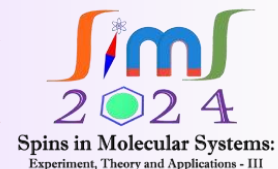
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## Spin Crossover System with Multifunction

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Spin crossover (SCO) compounds with multi-functions are attracting attention because of its switching property. We have also investigated photo switching, thermochromism, luminescence, conductivity, gas adsorption, liquid crystal, ferroelectricity, single molecule magnet in SCO systems. Ferroelectrics that display electrically invertible polarization are attractive materials because of their potential for wide-ranging applications. To date, considerable effort has thus been devoted towards developing ferroelectric materials, particularly those comprising organic/inorganic compounds. In these systems, structural dynamics such as atomic displacement and reorientation of polar ions/molecules play a key role in the generation of reversible spontaneous polarization. Although there are many reports concerned with organic/inorganic ferroelectrics, ferroelectrics based on coordination metal complexes have been largely unexplored despite their often unique electronic and spin state properties. In this feature article, we discuss recent progress involving coordination metal complex-based ferroelectrics where the reversible polarization originates not only from structural dynamics (represented by proton transfer, molecular motion, and liquid crystalline behavior) but also from electron dynamics (represented by electron transfer and spin crossover phenomena) occurring at the metal center. Furthermore, unique synergy effects (i.e., magnetoelectric coupling) resulting from the structural and electron dynamics are described. Recently, we also focused on spin qubit behavior as a multi-functional SCO. In this presentation, I would like to discuss on multi-functional SCO.



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## Probing the magnetic properties of actinide complexes by paramagnetic NMR

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The paramagnetic NMR (pNMR) chemical shift of a given nucleus is the difference between the observed shift and the shift observed for a diamagnetic analogue. This shift may be split into a *dipolar* term, arising from the magnetic dipolar interaction between the metal center and the NMR active nucleus, and a *contact* term, due to the spin delocalization leaking from the paramagnetic center towards the ligand.<sup>1</sup>

In this presentation, I will first discuss how this pNMR shift can be calculated with first principle methods, either CAS based or DFT.

Then, I will illustrate the diversity of information provided by pNMR chemical shifts measured on different nuclei of the ligands coordinated to actinide cations, the so-called Actinide Induced Shifts (AIS).

In complexes with a strong anisotropy, it gives access to the anisotropic magnetic susceptibility  $\Delta\chi$ .<sup>2,3</sup> 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.<sup>3,4</sup> The pathway of the spin density from the magnetic 5f orbitals to the nuclei will be discussed.

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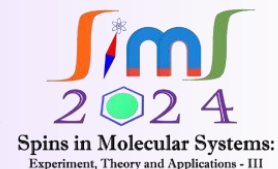
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## Speakers for Day 3 : 7<sup>th</sup> November 2024

- 1) Arindam Ghosh
- 2) Alessandro Lunghi
- 3) Masayuki Nihei
- 4) Vinod C. Prabhakaran
- 5) Swapan Pati
- 6) Dawid Pinkowicz
- 7) Ehesan Ali
- 8) Yanling Li
- 9) Kuduva R Vignesh
- 10) Naitik Panjwani
- 11) Sandeep K. Gupta
- 12) Daniel Talham
- 13) Peter Comba
- 14) Hitoshi Miyasaka
- 15) Tomohiro Takayama
- 16) Mario Ruben
- 17) Aaron Mailman
- 18) Fernando Luis
- 19) Pierre Dechambenoit
- 20) Pramod Bhatt
- 21) Eliseo Ruiz
- 22) Pradip K. Chakraborty
- 23) Matthew P. Shores
- 24) Masanori Wakizaka
- 25) Arup Sarkar (ERL)
- 26) Abinash Swain (ERL)
- 27) Krishna Kaushik (ERL)
- 28) Swapnil Shukla (ERL)
- 29) Lorenzo Sorace
- 30) Satyaprasad P. Senanayak





## Engineering interfaces in metals for strong charge-lattice-spin coupling

Arindam Ghosh

Engineering strong electron-lattice coupling can have many effects, ranging from superconductivity, to the formation of polarons – a collective state of conduction electrons and lattice vibrations or phonons. Usually materials with strong electron-phonon coupling are complex, both electronically and structurally, and addressing 'the polaron problem' can benefit from a simpler material platform. In this talk I shall outline a new nanostructuring strategy of crystalline Au within which we embed a distributed network of ultra small silver nanoparticles (AgNPs) of radius  $\sim 1 - 2$  nm. This hybrid structure exhibits an unprecedented enhancement in the electron-phonon interaction, with effective coupling constant  $\lambda$  as high as  $\approx 20$  that is  $\sim$  hundred times that of Au and  $\sim$  ten times larger than any known metal. Remarkably, the temperature-dependence of the electrical resistivity above the Debye temperature in these hybrids deviates from linearity at high AgNP density and approaches a saturation to the Mott-Ioffe-Regel scale. We will also show that such a dense network of interfaces leads to enhanced spin-orbit scattering through an emergent Rashba effect.



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## Computational Design of Magnetic Molecules

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Magnetic molecules have been proposed for many different applications, including acting as quantum sensors, spintronics elements, memory storage units and much more. Unfortunately, only a few candidates at best are known to retain their spin orientation and coherence at a relevant temperature for such applications. Now that a robust ab initio theory of spin decoherence for magnetic molecules have been developed, a clear list of requirements necessary to support long spin coherence and lifetime is available [1,2] and only awaits to be implemented. However, identifying an actual compound that embeds all the right requirements remains a critical challenge.

In this contribution, I will describe how theory and ab initio computational tools can be integrated in such a way that the entire design process of magnetic molecules with ideal properties is streamlined and automatic [3]. A case study on Co(II) single molecule magnets is presented. Around 22,000 chemically-diverse single-ion coordination compounds are automatically assembled from a list of predefined organic ligands extracted from the Cambridge Structural Database. All these compounds are then optimized with Density Functional Theory to reveal around 16,000 stable molecules. The latter are then screened with Complete Active Space Self Consistent Field to estimate their magnetic anisotropy, the leading contribution to long spin lifetime in this class of single-molecule magnets. The entire methodology is automatized and able to run on high-performance computing machines with minimal user intervention. Tens of new molecules with  $|D| > 100 \text{ cm}^{-1}$  have been identified, including some with  $|D| > 230 \text{ cm}^{-1}$ , thus comparable to the record value for Co(II) SIMs [4]. Ongoing future developments for this computational strategy, its strengths and limitations will be discussed.

**Acknowledgments:** European Research Council (ERC): grant agreement no. [948493].

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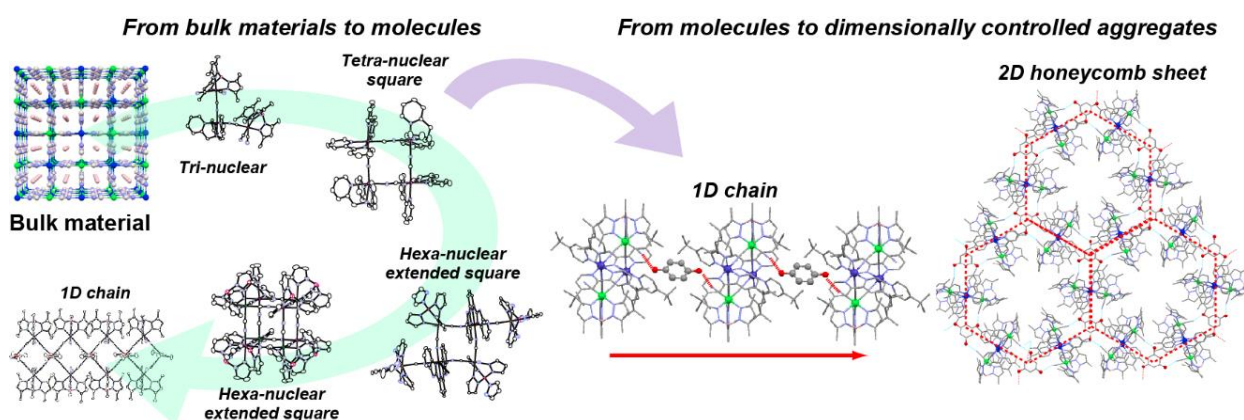
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# Molecular Prussian Blue Analogues: From Bulk to Molecules and Low-dimensional Aggregates

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Physical functions of bulk materials originates from their infinite electronic structures with large degree of freedom of electrons, spins and phonons. On the other hand, molecules have discrete energy levels and flexible molecular- and electronic-structures, and precise control of their frontier energy levels leads to a specific molecular functions. Prussian blue analogues (PBAs) are three-dimensional bulk solids constructed by bridging cyanide and metal ions. CoFe PBA has been reported to show light-induced magnetization based on an electron-transfer-coupled spin transition (ETCST). Discrete cyanide-bridged multi-nuclear clusters can be considered as zero-dimensional PBAs. We have prepared a series of cyanide-bridged multi-nuclear clusters, and we report here controlled ETCST by external physical- and chemical-stimuli.<sup>1)-3)</sup> In addition, dimensionally controlled assemblies of the cyanide-bridged clusters with multi-stability will be presented.<sup>4)-8)</sup>



**Figure 1** Cyanide-bridged multinuclear clusters as a functional unit of bulk PBA (left), and their low-dimensional aggregates (right).

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## Nailing the Holy Grail of Methane Partial Oxidation

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Direct methane partial oxidation and its conversion to fuels and chemicals is considered one of the holy grail problems in Catalysis<sup>1</sup>. With all the C-H bonds very stable and weakly polarizable, an indirect route where synthesis gas (CO+H<sub>2</sub>) and its downstream processing through FT synthesis or methanol synthesis is the only mature downstream technology available. In this lecture I will present how novel catalyst design can result in efficient direct conversion of methane to methanol and formic acid<sup>2-4</sup>. The talk will also cover the mechanistic details of the correlation between structure and activity that leads to oxygenates.

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## Computational Modeling of Competing Magnetic Phases, Quantum Spin Liquid Candidates and Molecular Magnets

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After a brief introduction to fundamentals of quantum magnetism, I shall discuss on 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 DM interactions. The linear spin-wave theory and density matrix renormalization group (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 [1]. I shall also discuss the possible quantum spin liquid phases in dimer-based material,  $\text{Yb}_2\text{Te}_5\text{O}_{13}$  and hyperhoneycomb random lattices,  $\text{NaYbW}_2\text{O}_8$  with two compositions, which were synthesized and thermodynamical and m-SR studies were carried out by our experimental colleagues [2]. In fact, after finding the exchange constants, single ion anisotropy and biaxial anisotropy, our Monte Carlo based prediction of incommensurate phases at certain temperatures for all the spin lattice systems. In fact, since the neutron scattering data is missing, we have verified our results with the experimental m-SR data. Many more detail experimental and quantum theoretical studies are necessary to identify these as the elusive quantum spin liquid candidates [2]. Thereafter, I shall discuss a few molecular magnets based on Fe4 and Dy systems and their probability of corresponding tunnelling versus hopping mechanisms [3]. Finally, I shall show the nonlinear magneto-electric effect in a toy model (finite size spin-orbital lattice) with tuning the Hubbard and spin-orbit coupling interactions [4].

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# REVERSIBLE PHOTOCHEMISTRY AND MAGNETISM OF CYANIDE-BRIDGED MOLECULAR SOLIDS

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Photochemical processes are widely studied due to the abundance of visible light photons provided by the Sun and the possibility of developing 'greener' alternatives to current technologies. When it comes to the control of the magnetization by photons – the so called photomagnetic effect – there are examples among molecular materials showing light induced excited spin state trapping (LIESST)<sup>1</sup> or even among conventional solids such as rare-earth orthoferrites demonstrating light-induced ultrafast spin reorientation.<sup>2</sup> However, the use of photochemical reactions to exert reversible photomagnetic switching in the solidstate is rare. Herein, we will demonstrate and discuss the advantages and challenges of employing photochemical reactions in the design of photomagnetic solids. In particular, the light-driven cyanide dissociation/association in a single crystal of potassium heptacyanomolybdate(III) dihydrate will be presented as the representative example of this strategy. Moreover, the use of this and related building blocks in combination with other paramagnetic species will be demonstrated, leading to a significant switching of the magnetic ordering.<sup>3,4</sup>

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# Exchange Interactions Induced Magnetization Relaxation in Single Molecule Magnets

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Lanthanide single-molecule magnets (SMMs) incorporating organic ligands with unpaired radical electrons have emerged as promising candidates for molecular-scale device applications.[1,4] The magnetic exchange coupling between the ligand's delocalized spin density and the lanthanide's localized magnetic moment is pivotal in suppressing low-temperature demagnetization and facilitating complex, slow magnetic relaxation at moderate to high temperatures. In this study, we have investigated the demagnetization mechanism of Terbium (III) bis-phthalocyanine double-decker [TbPc<sub>2</sub>]0 complexes, focusing on the influence of the ligand radical electron. Employing wavefunction-based multireference ab initio calculations, we have analyzed the 4f- $\pi$  radical exchange coupling and the Tb(III) ion's magnetic moment reversal pathways. Our results demonstrate that the Ising-type exchange coupling splits the single-ion ligand field manifold sublevels into Kramers pairs, enabling multiple channels for Tb(III) magnetic moment flipping. This finding offers a promising avenue for controlling magnetization relaxation by fine-tuning intramolecular exchange interactions.[5] items

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# Cyanide-bridged Fe<sub>2</sub>Co<sub>2</sub> tetranuclear complexes - Contribution of pressure study to the comprehension of magnetic switching

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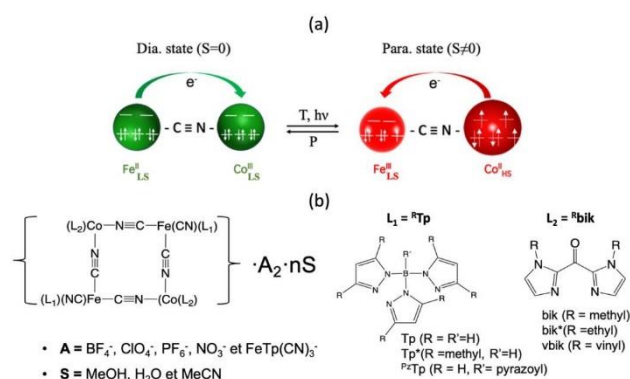
[Yanling.li@sorbonne-universite.fr](mailto:Yanling.li@sorbonne-universite.fr) and [Rodrigue.lescouezec@sorbonne-universite.fr](mailto:Rodrigue.lescouezec@sorbonne-universite.fr)

Over the last two decades, bistable molecular counterparts of FeCo Prussian Blue Analogues (mPBAs) have attracted increasing attention as molecular magnetic switches. Under external stimuli such as light, temperature, pressure, electric field, these cyanide-bridged coordination clusters can undergo intramolecular electron transfer - coupled to a spin transition on the cobalt site (ETCST), converting thus the (Fe<sup>II</sup><sub>LS</sub>-CN-Co<sup>III</sup><sub>LS</sub>) state into (Fe<sup>III</sup><sub>LS</sub>-CN-Co<sup>II</sup><sub>HS</sub>) one (schema 1a).<sup>1,2</sup>

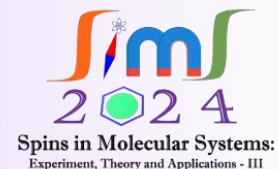
Numerous efforts have been focused on the control of the light-induced and thermally-activated ETCST process in the solid state, while pressure study has been somewhat neglected. However, pressure as stimulus has been successively used to tune the switching process of Fe(II) based spin transition compounds.<sup>3</sup> The cyanide-bridged Fe<sub>2</sub>Co<sub>2</sub> complexes are the most studied FeCo coordination clusters reported in the literature.<sup>4</sup> They have the general formula {[Fe(<sup>R</sup>Tp)(CN)<sub>3</sub>]<sub>2</sub>[Co(L)<sub>2</sub>]<sub>2</sub>}(A)<sub>2</sub>·S, where <sup>R</sup>Tp = tris(pyrazolyl)borate derivatives, L = α-diimines, A = counter-anion and S = solvent. Since 2009, our group has conducted studies on the ETCST of square complexes with bis(imidazolyl)ketone derivatives (β-diimines) as capping ligands on the Co ion. These compounds feature different ligand substitutions, counter-anions and solvents (schema 1b). We have used light, temperature and especially pressure as external stimuli.<sup>5-8</sup>

This presentation will cover the selected results focusing on two main topics:

1. the structure-property relationship of the Fe<sub>2</sub>Co<sub>2</sub> square complexes.
2. the contribution of pressure study to the comprehension of the magnetic switching of polymeric complexes.



Schema 1. (a) Electron transfer coupled spin transition in FeCo coordination clusters and (b) Cyanide-bridged tetranuclear Fe<sub>2</sub>Co<sub>2</sub> complexes prepared at IPCM laboratory.



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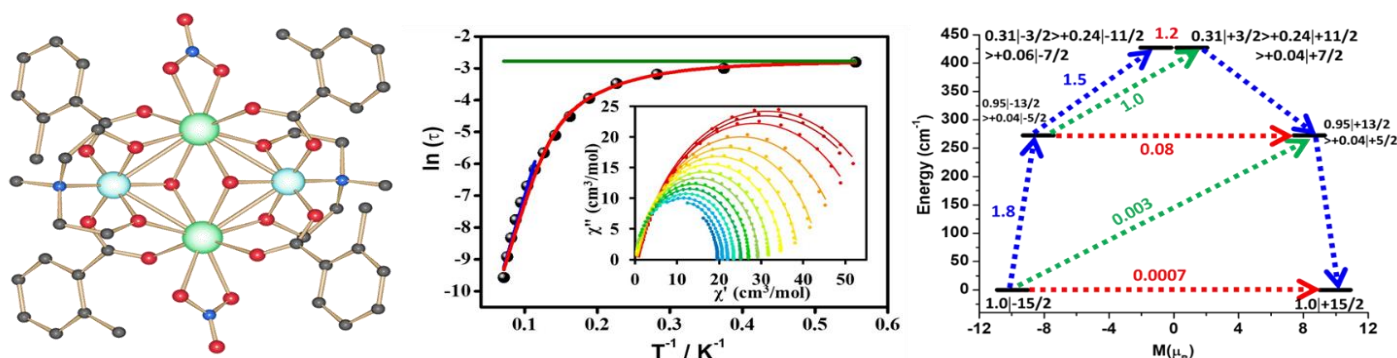
# Role of 3d/4d-4f magnetic exchange interactions and diamagnetic 3d ions on the Ln(III) magnetic dynamics in heterometallic {3d/4d-4f} SMMs

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Single-molecule magnets (SMMs) are discrete molecules that display magnetic hysteresis below a certain temperature.<sup>1</sup> 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.<sup>2</sup> 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 (*ab initio* and DFT) to understand their molecular magnetic behavior will be discussed. Single-ion Dy(III) examples were made in our lab to show large thermal anisotropy barriers to magnetic reversal. The effect magnetic exchange has on the SMM properties of dinuclear Ln complexes and several heterometallic 3d-4f/4d-4f complexes have been probed. 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.<sup>3</sup>



**Figure.** (left) Molecular structure of {Ru<sup>III</sup>}\_2Ln<sup>III</sup>}\_2 SMM; (middle) Magnetization relaxation time ( $\tau$ ), plotted as  $\ln(\tau)$  vs.  $T^{-1}$  for a {Dy<sup>III</sup>}\_2 SMM. (Inset) Cole–Cole plots between 1.8 and 14 K. (right) *Ab initio* computed magnetic relaxation of a {Co<sup>III</sup>}\_2Dy<sup>III</sup>}\_2 complex.

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## Optically addressable spin states in fully organic diradicals probed by spin resonance techniques

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Molecular systems are promising candidates for quantum information technologies due to their reproducible nature and chemical tailorability. One particularly promising platform is spin radical organic semiconductors, which can exhibit high luminescence<sup>1,2</sup> and show spin dependent luminescence via high spin states<sup>3</sup>.

The work presented here<sup>4</sup> involves the study of a family of TTM based diradical systems which are linked together via either a strong or weak electron donating group. The diradicals are studied using electron paramagnetic resonance (EPR) spectroscopy, which reveals spectral signatures consistent with a triplet dark-ground state. Transient EPR results show a strong ground state spin polarisation persisting up to 200  $\mu$ s at 200 K for one diradical system, arising from spin-sublevel selective intersystem crossing. Using pulsed EPR we show coherent manipulation of the spin state and the measured spin coherence times. We further explore optical initialization and read-out of spin-states via optically detected magnetic resonance (ODMR) spectroscopy.

The diradicals presented here provide new possibilities for room temperature optically addressable qubits, via an all-organic molecular spin semiconductor.

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arxiv.org/abs/2406.03365



## Maximizing the Magnetic Anisotropy in Four-Coordinate Cobalt(II) Single-Ion Magnets

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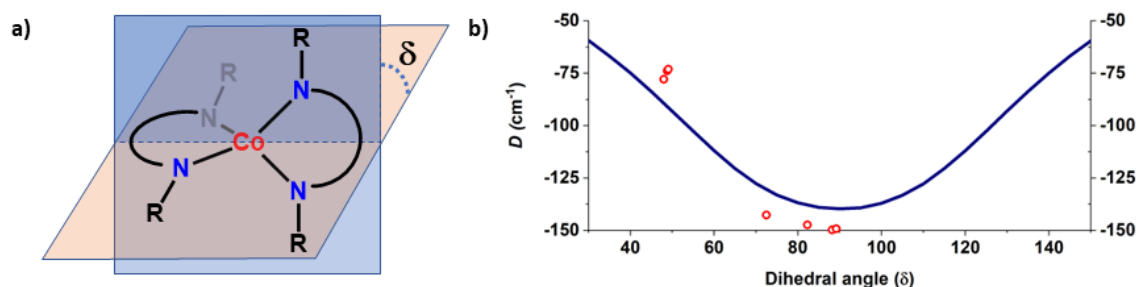
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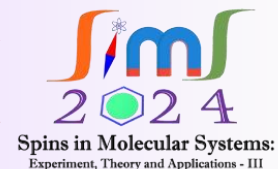
A comprehensive understanding of the ligand field and its influence on the degeneracy and population of *d*-orbitals in a specific coordination environment are crucial for the rational design and enhancement of magnetic bistability.<sup>1-2</sup> Research on 3d-single-ion magnets (SIMs) has revealed that a large negative zero-field splitting (*D*) besides a high-spin ground state (*S*) is the essential requirement to realize a high anisotropic energy barrier ( $U_{\text{eff}}$ ) for slow magnetization reversal. To add further understanding of the underlying factors that affect magnetic anisotropy, we have investigated a family of four-coordinate dianionic mononuclear Co(II) complexes with the general formula  $[\text{L}_2\text{Co}][\text{X}]_2$  (where L is a diamido ligand and X are counteranions). These complexes exhibit a pronounced variation in the magnetic anisotropy which can be directly correlated to the local dihedral angle ( $\delta$ ) (Figure 1). The study further shows that slow magnetic relaxation can be switched “on” and “off” by carefully manipulating the dihedral angle.<sup>3</sup> A combination of single-crystal synchrotron X-ray diffraction for the determination of experimental electron density (EED) and polarized neutron diffraction (PND) that quantifies the magnetic anisotropy provides key information about *d*-orbital populations and the magnetic anisotropy tensor.<sup>4</sup> We will also present a strategy to enhance the SIM properties of 3d metal complexes with hard O-donors by modulating the ligand field character via the coordination of diamagnetic ions and the benefit of robust metalloligands in that regard.<sup>5</sup>



**Figure 1.** (a) Schematic representation of  $[\text{L}_2\text{Co}][\text{X}]_2$  core elucidating the dihedral angle ( $\delta$ ). (b)  $D$  plotted as a function of the dihedral angle. The blue line shows the CASSCF calculations with rotated geometries starting from an idealized  $D_{2d}$  geometry.

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## Interface and Matrix Effects on Spin Transition Solids

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If switchable spin-transition magnetic networks are to be incorporated into complex architectures for applications ranging from spintronics to mechanical actuators, the ways in which their behavior changes at surfaces or when coupled to other components must be understood. For example, when spin-transition materials are incorporated into thin-film or core-shell particle heterostructures, thermally- or optically-induced spin state changes couple across the interface to change the behavior of the second material. At the same time, the response of the spin-transition network also changes. Spin transitions alter metal-ligand bond distances leading to large volume changes, as high as 10-15%, resulting in significant coupling of the magnetic and elastic properties. This presentation will highlight recent results of spin-transition solids in core-shell particles, multicomponent thin films and 2D-3D heterostructures, showing how heterostructure behavior is influenced by the solid-solid interface and solid-state elastic properties of each component.



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## Modeling Spin for Applications of Metal Complexes

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Unpaired electrons are of importance for the reactivity of transition metal complexes and are responsible for spectroscopic and molecular magnetic properties of transition metal and rare earth compounds. Thorough experimental studies combined with quantum-chemical modeling help to optimize systems for specific applications. Three examples are presented to demonstrate the relation between coordination geometry and electronic structure: (i) The activation of oxygen by high-valent nonheme iron complexes, where the efficient modulation of the energy gap between the spin ground and first excited states lead to the most reactive iron(IV)oxido catalyst known to date.<sup>1,2</sup> (ii) A manganese(II) based MRI contrast agent with exceptional stability, manganese(II) selectivity and MRI efficiency.<sup>3,4</sup> (iii) The validation of ab-initio predicted magnetic anisotropies in dysprosium(III) compounds.<sup>5-7</sup>

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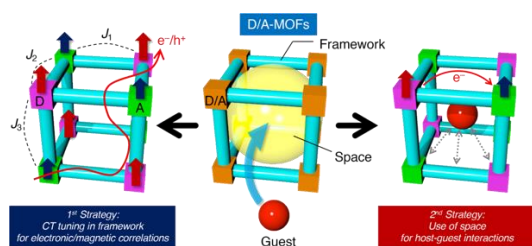
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## Magnetic Sponges for Switching

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Creating materials with a range of sensing capabilities that can be manipulated by chemical and physical stimuli is a significant challenge in materials science. A class of metal-organic frameworks (MOFs), known as electron-conjugated framework materials consisting of electron-donors (D) and/or -acceptors (A), is a promising candidate for such applications [1,2]. This class of materials, which we refer to as "D/A-MOFs", allows for the tunable charge transfer (CT) of  $D^0A^0 \leftrightarrow D^{\delta+}A^{\delta-}$  based on the parameters of the ionization potential of D and electron affinity of A, as well as Madelung stabilization of the ionic  $D^+A^-$  set, and can be sensitive to stimuli. Thus, D/A-MOFs are intriguing targets for guest-sensitive functional materials with electronic, magnetic, and dielectric properties as well as their porous nature for gas/solvent sorption or ionic transportation. Multidimensional frameworks were designed using paddlewheel-type diruthenium(II, II) complexes ( $[Ru_2^{II,II}]$ ) as D and TCNQ or DCNQI derivatives as A, and the ability to control CT in D/A-MOFs to achieve electronic and magnetic functionalities has been demonstrated [2]. The magnetic properties of porous  $D_2A$  layered systems with void spaces between layers are highly responsive to interlayer environments, which are relevant to guest molecules that are present or inserted between layers, and often impact the charge-ordered state of the materials [3–12].



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## Development of candidate materials for Kitaev spin liquid

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Quantum spin liquid (QSL) where interacting spins remain disordered down to zero temperature represents a novel quantum state of matter hosting fractionalized excitation. Kitaev honeycomb model with bond-dependent Ising magnetic interactions is considered as a promising avenue for realizing a QSL state [1]. Honeycomb transition-metal compounds with strong spin-orbit coupling, such as  $5d$  iridates and  $4d$   $\text{RuCl}_3$ , have been proposed to display such bond-dependent magnetic interactions [2], but most of candidate materials were shown to undergo long-range magnetic order, instead of spin-liquid state. This is likely due to the presence of additional non-Kitaev magnetic interactions [3]. The realization of Kitaev spin liquid calls for further materials exploration.

We found that the protonated honeycomb iridate,  $\text{H}_3\text{LiIr}_2\text{O}_6$ , shows no magnetic order or spin-glass freezing down to 50 mK, despite strong magnetic interactions inferred from the Curie-Weiss temperature of -100 K, indicating a quantum spin liquid state [4]. However, any experimental evidence for Kitaev-type QSL is lacking so far and the driving force for the QSL state remains elusive. We focused on the critical role of  $\text{H}^+$  ions between the Ir honeycomb layers, and examined the isotope effect by synthesizing  $\text{D}_3\text{LiIr}_2\text{O}_6$ . While substantial isotope effect on magnetic interactions was identified in  $\text{D}_3\text{LiIr}_2\text{O}_6$ , the QSL ground state was found to be robust. We argue that the disorder of  $\text{H}^+/\text{D}^+$  positions likely gives rise to bond-disorder in magnetic interactions and stabilizes a QSL state.

In addition to  $5d/4d$  systems,  $3d$  cobaltates have recently appeared as a new platform of Kitaev physics. We will also discuss our exploration for honeycomb-based cobaltates which may realize Kitaev-type spin liquid state.

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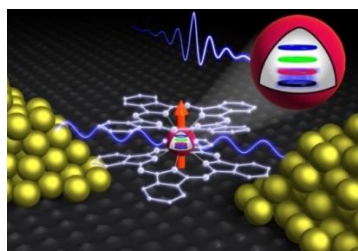
## Quantum Computing with Molecules

Mario Ruben

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Metal complexes will be proposed to act as active quantum units for Quantum Computing (QC). We report on the implementation of metal complexes into nanometre-sized (single-)molecular spintronic devices by a combination of isotopologue chemistry, bottom-up self-assembly and top-down lithography techniques. The control of the Hilbert space of the molecular quantum magnets on conducting surfaces/electrodes will be shown and persistence of magnetic properties under confinement in Supramolecular Quantum Devices (SMQD) will be proven. The quantum behaviour (e.g., superposition) of the metal complexes will be addressed at the single molecule level<sup>1-13</sup> to finally implement a quantum algorithm on a TbPc<sub>2</sub>-Qudit performing quantum computing operations.<sup>10</sup> Moreover, we will show that the components of SMQDs as the Quantum Magnet<sup>14</sup> and the graphene sheets<sup>15</sup> can be made from CO<sub>2</sub> guaranteeing a negative Carbon footprint and sustainability of the molecular approach towards QC.



**Figure 1** Artistic representation of a Molecular Spin Transistor based on a TbPc<sub>2</sub> complex acting as a molecular Spin Qudit.<sup>8</sup>

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### Recent Reviews:

"Molecular Spin Qudits for Quantum Algorithms."

E. Moreno-Pineda, C. Godfrin, F. Balestro, W. Wernsdorfer, M. Ruben  
*Chem. Soc. Rev.* **2018**, *47*, 501.

„Synthetic Engineering of the Hilbert Space of Molecular Qudits: Isotopologue Chemistry.“

W. Wernsdorfer, M. Ruben  
*Adv. Mat.* **2019**, *31*, 1806687.



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## Achieving Thermal Hysteresis in Neutral and Ionic Main Group Radicals

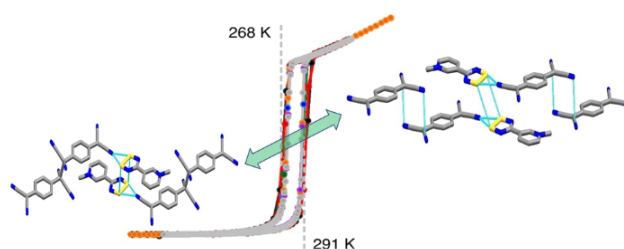
Aaron Mailman,<sup>a\*</sup> Ankita Naik,<sup>a</sup> Juho Toivola,<sup>a</sup> Manu K. Lahtinen,<sup>a</sup> Sebastien Bonhommeau,<sup>b</sup> Itziar Oyarzabal,<sup>c,d</sup> and Rodolphe Clérac<sup>e</sup>

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Molecules that display dynamic covalent-bonding characteristics in response to external stimulus (heat, light, pressure, etc), such as, crystalline organic radicals, have attracted considerable attention for application as electronic and information storage devices [1,2]. The observation of magnetic bistability in organic radicals still remains relatively rare compared to the closely related spin-crossover (SCO) phenomenon observed in some metal complexes. While the SCO phenomenon occurs by a spin transition between a high-spin (HS) and low-spin (LS) state [3], organic radicals undergo an interconversion between a radical ( $S = \frac{1}{2}$ ) and its  $\pi$ - or  $\sigma$ -dimer ( $S = 0$ ) because of perturbations in one or more external stimuli. These reversible solid-state to solid-state (or liquid state) transitions can be structurally studied by single crystal and/or powder X-ray diffraction methods and the different electron-exchange interactions of the phases give rise to hysteresis loops in the magnetic susceptibility.

Several different strategies have recently been utilized to sterically or electronically stabilized molecules so that they display a bistable regime controlled by the molecular and/or solid-state structure. An overview of recent developments in main-group radical-based materials displaying thermal hysteresis will be discussed.



**Figure 1.** Temperature dependence of the  $\chi T$  product between 1.85 – 380 K at 1 T with different heating and cooling rates for the phase transition between a TCNQ  $\sigma$ -dimer dianion and two TCNQ radical-anions in a organic radical-ion salt (Sulfur = yellow, Nitrogen = blue, Carbon = grey; Intermolecular interactions = light-blue dashed lines).

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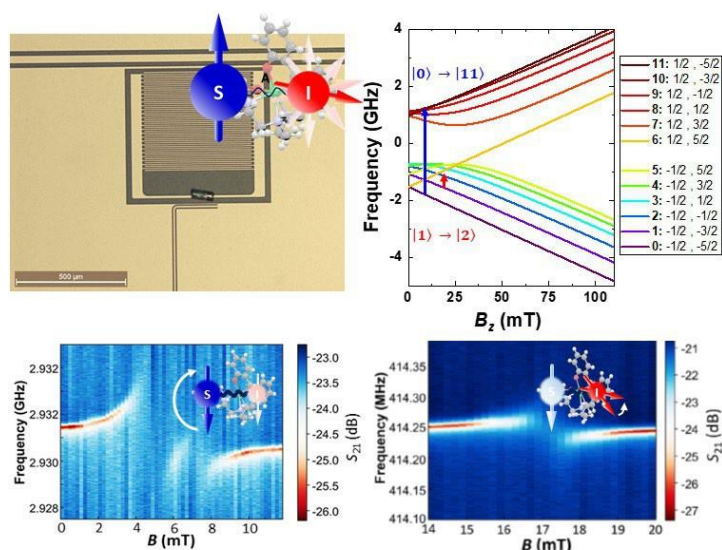
## Wiring up Molecular Spin Qudits with Superconducting Circuits

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Scaling up quantum processors remains very challenging, even for today's most successful platforms. Molecular complexes able to encode  $d$ -dimensional qudits in their electronic and nuclear spin states can act as universal quantum processors or even correct errors [1]. I'll discuss recent experiments aimed at exploiting these systems by coupling them to superconducting resonators [2,3]. A high cooperativity coupling to electronic and even nuclear spins has been achieved [3,4]. We also find that it is possible to couple excitations of remote, and distinct, spin ensembles by means of interactions mediated by the circuit. The results provide the basis for the control, readout and communication of spin qubits and qudits and for implementations of quantum algorithms.



**Figure 1** A single crystal of  $^{173}\text{Yb}$ trensals, which hosts an electronic spin qubit and a  $d = 6$  nuclear spin qudit, is coupled to a superconducting resonator. Microwave transmission experiments show that the spin-photon coupling reaches high cooperativity, which allows reading out the qudit states.

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## How and why promoting large spin delocalization in molecule-based magnets?

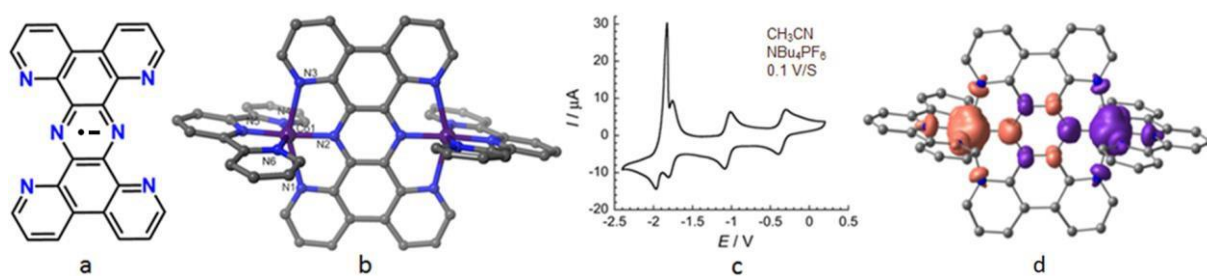
X. Ma,<sup>a</sup> M. Suo,<sup>a</sup> D. Lou,<sup>a</sup> E. A. Suturina,<sup>b</sup> N. Yutronkie,<sup>a</sup> M. Rouzières,<sup>a</sup> A. Rogalev,<sup>c</sup>  
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**Molecular engineering** can be defined as the design of molecules or molecular assemblies whose architecture must enable to fulfill a function.<sup>[1]</sup> Historically developed for pharmaceutical sciences, this reasoned “bottom-up” approach is now applied into various fields such as photovoltaics, synthetic biology, energy or gas storage (batteries, MOFs...). It can operate at nanometric and macroscopic scales (materials), and is taking advantage of the concepts and synthetic tools developed in molecular and supramolecular chemistries. This rational and elegant approach is also particularly attractive for the design of molecular architectures with preconceived and controlled magnetic properties. Through the **experimental study** of a series of prototypes of dinuclear complexes (Figure),<sup>[2]</sup> we will see: i) what are the factors which govern the strength and sign of the magnetic exchange interaction through an aromatic ligand, and ii) how to promote electronic delocalization, a prerequisite for the rational design of molecular conductors and/or magnets at high temperatures. A couple of **room temperature molecule-based magnets** will then be discussed.<sup>[3]</sup>



**Figure.** a) Tetrapyrrophenazine (tphz\*) radical bridging ligand ; b) Crystal structure of the complex  $[\text{Co}_2(\text{tphz}^*)(\text{terpyridine})_2]^{3+}$ ; c) Cyclic voltammogram and d) spin density distribution in the same complex.

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## Prussian Blue Analogues Molecular Magnets: Pigments to Power

Pramod Bhatt

Solid State Physics Division

Prussian blue analogues (PBAs), initially valued for their distinctive blue pigment, have recently gained prominence as multifunctional materials with a wide range of technological applications. From gas storage to serving as electrode materials for batteries and supercapacitors, as well as applications in environmental and biomedical fields, PBAs are now at the forefront of cutting-edge research. In this presentation, I will delve into our R&D efforts on molecular magnets, exploring their structural and magnetic properties, and the diverse applications [1-5]. I will discuss recent advances in the synthesis, characterization, and functionalization of PBAs, demonstrating how these materials can be engineered to suit specific technological needs. By examining the underlying physics and materials chemistry that enhance their functionality, we aim to highlight the role of PBAs in contributing to sustainable energy solutions and other technological innovations. Our research underscores the vast potential of these versatile materials for a wide array of future applications.

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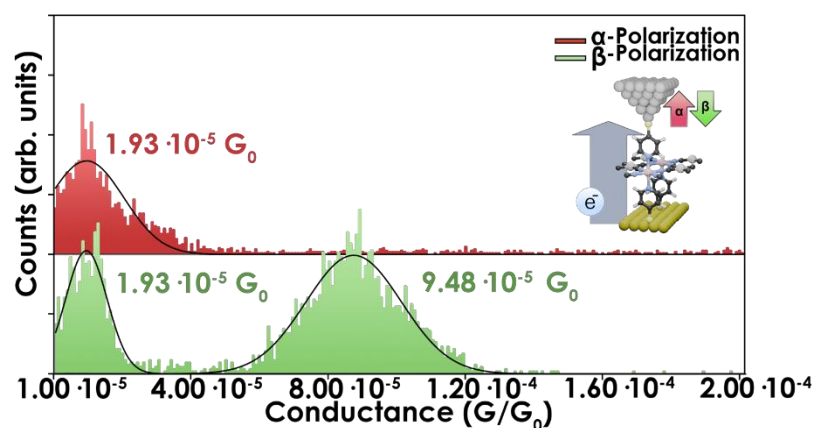


## From Single-Molecule to 2D Layers: Magnetism and Transport

Eliseo Ruiz

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Magnetic molecules can provide surprising behaviors, especially in single-molecule level properties. In this presentation, I will show the results of a spin-crossover system in which a single molecule can exhibit hysteresis. This behavior was not expected because, usually, the hysteresis was related to intermolecular cooperative interactions. In this case, the blocking of one of the molecule's spin states occurs, generating a hindrance in the spin transition that opens the hysteresis loop.[1] A second part will be devoted to measurements of transport properties through magnetic systems using a scanning tunneling microscope (STM). Some magnetic systems present magnetoresistance effects in break junctions at room temperature. This effect appears when using a magnetic electrode, changing the direction of the magnetization of that electrode produces a change in the conductance across the magnetic system located at the junction. This behavior has been analyzed from single-molecule systems[2,3] to 2D layers devices based on Hofmann clathrate hosts (see Fig. 1).



**Figure 1** Histograms of STM Conductance values for the  $[\text{CoPt}(\text{CN})_4]$  system using Et-S-S-py as anchoring ligand to the substrate and a functionalized Ni tip with mercaptopyridine. The transport properties with two magnetizations of the Ni tip (red and green arrows).

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## Unraveling Structure-property Interplay in Fe(II) and Co(II) Spin-crossover Coordination Networks: A Fascinating Diversity

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Spin-crossover (SCO) coordination networks are unique molecular systems showing modification of their spin state configuration. The SCO phenomenon involves reversible stimuli-responsive and composition-specific switching between two electronic configurations stemming from the reorganization of electrons within transition metal d-orbitals between the high-spin (HS) and the low-spin (LS) states, yielding maximum and minimum number of unpaired electrons, respectively. The molecular-level switching (i.e., short-range in nature) can be generally understood through chemically governed ligand-field tunability, degree of covalency, and non-covalent interactions, for instance,  $\pi$ - $\pi$  or hydrogen bonding interactions. Whereas, the macroscopic switchability (i.e., long-range) is usually explained by the degree of electron-phonon coupling mediated by the elastic interactions within the crystal lattice leading to the so-called cooperative effects, and are well defined as a superposition of short- and long-range interactions. While undoubtedly cooperativity is an important property of SCO networks for practical applications, it is crucial to understand and design the cooperativity, in terms of controlling the hysteresis width, degree of completeness of the transition, and multistep behavior.

Therefore, fundamentally and from an application standpoint, it is essential to explore the stimuli-responsive structural diversity of the compositionally-tuned SCO coordination networks and their connection with the variation in SCO/magnetic properties with a focus on understanding the origin of cooperative effects (if any) for the designing of functional materials useful for the construction of sensors, spintronic and memory devices. Accordingly, in the present talk, I will discuss the detailed stimuli-responsive structures and associated magnetic and photophysical behavior in combination with the theory for selected Fe(II) and Co(II)-based SCO coordination networks.



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## Elucidating and controlling intermolecular interactions for magnetic switching

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Spin crossover and single-molecule magnetism are molecular-level manifestations of delicately balanced electronic states. Both are challenging to predict computationally, so there is a strong role for synthesis and characterization of new species to elucidate and eventually control magnetic properties. In the first part of the seminar, we will focus on controlling spin state in Fe(II) complexes via post-synthetic modification of complexed ligands, toward developing “simple” predictive models for spin-crossover propensity. In the second part of the seminar, we will explore single-molecule magnet properties of  $S = 1/2$  coordination complexes of Ni(III) and Co(II) ions, which in principle represent the simplest electron-based quantum bits (qubits) for developing molecular quantum computers. In both cases, teasing apart the intra- and inter-molecular interactions driving magnetic switching requires systematic variation of local ligand fields and intermolecular networks.



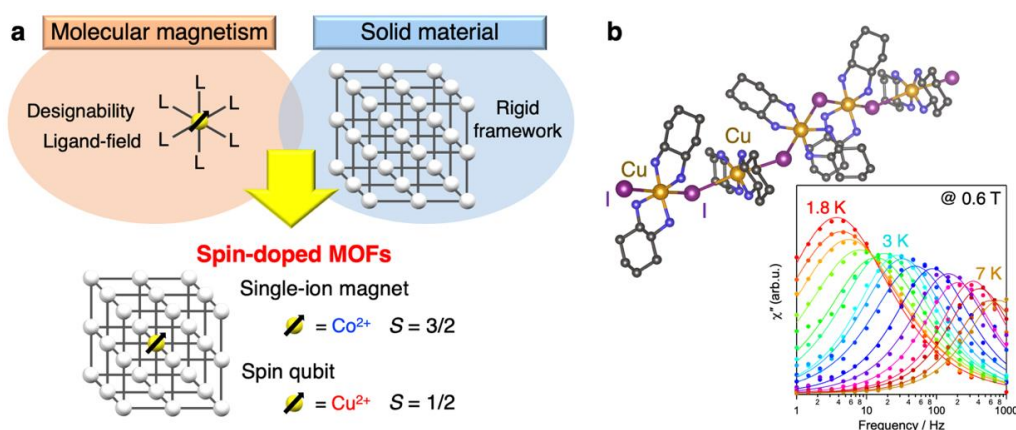
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## Quantum magnetism of Co(II) and Cu(II) centers in metal-organic frameworks and in molecular-chains

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This work demonstrates a new simple strategy for the synthesis of quantum magnetic metal-organic frameworks (MOFs) where a diamagnetic MOF is used as the framework into which the spin centers are doped (Figure 1a). The Co(II) centers with a  $S = 3/2$  spin state or the Cu(II) centers with a  $S = 1/2$  spin state are doped into  $[\text{CH}_6\text{N}_3][\text{Zn}^{\text{II}}(\text{HCOO})_3]$  MOF changing doping amount. The doped Co(II) centers show single-ion magnetism with a positive  $D$  term of zero-field splitting and slow magnetic relaxations under a static magnetic field.<sup>1</sup> On the other hand, the doped Cu(II) centers show slow magnetic relaxation under a static magnetic field, but it is not single-ion magnets but spin qubits. Pulse electron spin resonance spectroscopy reveals spin coherence properties with a Hahn echo decay time above microseconds.<sup>2</sup> Furthermore, this work revealed that a Heisenberg weak anti-ferromagnetic molecular-chain consisting of  $[\text{Cu}^{\text{II}}(\text{chxn})_2]\text{I}$  ( $\text{chxn} = 1R,2R$ -diaminocyclohexane; Figure 1b) exhibits slow magnetic relaxations under a static magnetic field. This Cu(II) molecular-chain can be considered as a model of the connecting spin qubits one-dimensional system. This work links a one-dimensional quantum spin system and a spin dynamics system.<sup>3</sup>



**Figure 1.** (a) Concept of spin-doped MOFs and (b) slow magnetic relaxation of  $[\text{Cu}^{\text{II}}(\text{chxn})_2]\text{I}$ .

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# Deciphering the Origin of Double Exchange and Magnetic Exchange in a [Fe<sub>3</sub>] Cluster using Density Matrix Renormalization Group (DMRG) Approach

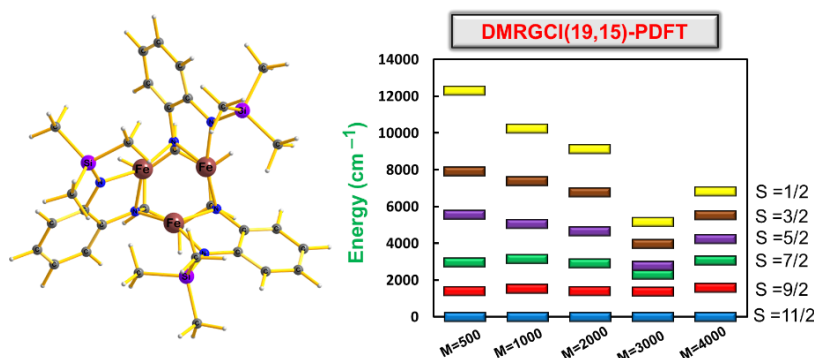
Arup Sarkar,<sup>a\*</sup> Neeraj Dhauni,<sup>b</sup> and Gopalan Rajaraman<sup>b</sup>

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Multinuclear metal clusters containing first-row 3d metal ions are promising to exhibit small molecule activation, biological electron transfer and magnetic memory devices. Particularly, mixed-valence iron clusters couple spin components via double-exchange and stabilize high spin states which displays excellent application towards single-molecule magnets.<sup>1,2</sup> Here by employing a combination of multireference methods such as Density Matrix Renormalization Group configuration interaction (DMRG-CI), multiconfiguration pair densityfunctional theory (MC-PDFT) and state average complete active space self-consistent field (SA-CASSCF) the spin ladder, double exchange and zero-field splitting of a mixed-valence trimeric iron cluster [(18-C-6)K(thf)<sub>2</sub>][(t<sup>bs</sup>L)Fe<sub>3</sub>] ((1,3,5-(<sup>t</sup>BuMe<sub>2</sub>SiNH-*o*-C<sub>6</sub>H<sub>4</sub>NH)<sub>3</sub>C<sub>6</sub>H<sub>9</sub>))<sup>3</sup> were identified. A very strong double exchange interaction with  $B = 230 \text{ cm}^{-1}$  was obtained from SA(14)-CASSCF(19,16) calculation which is in excellent agreement with the experimental maximum of  $\sim 250 \text{ cm}^{-1}$  from the intra-valence charge transfer (IVCT) band.



**Figure 1** Crystal structure of the [(<sup>t</sup>*bs*L)Fe<sub>3</sub>]<sup>-</sup> (left) and the DMRGCI-PDFT computed spinladder of the molecule (right).

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## Qubits Within Transition Metal Helicates: Encased Molecular Structures

Abinash Swain

The Molecular Qubits are a class of nano-magnets that are next-generation candidates for building quantum computers.<sup>1, 2</sup> The bit, which is embodied in a macroscopic physical object (such as a transistor or a magnetic domain) and can exist in two states, is the fundamental unit of information in classical computing. It encodes logical information as either 0 (up) or 1 (down). The quantum equivalent is a quantum entity known as a quantum bit or qubit, which has the two informational values represented as the quantum states  $|0\rangle$  and  $|1\rangle$ . The quantum physics laws that apply to qubits give resources that greatly increase the computational capacity. Every technology must meet a number of characteristics in order to offer eligible qubit candidates. The capacity to initialize the qubit state, scaling, the potential to correlate the quantum information among qubits, addressability, and, most significantly, extended coherence times in order to retain the quantum information are among these. Many various systems have been considered and researched, each of which has pros and cons in regard to those needs. In fact, it provides extremely significant benefits that elevate it to a serious player in the process of implementing QC, particularly the electronic spin. The most important parameters which affect the performance of molecular qubits or requirements to improve its performance are: i) low-spin complexes with small anisotropy (first-row transition metals with small spin-orbit contributions instead of heavier transition metals, such as rare-earth complexes), ii) metal centres carrying zero nuclear spins (such as  $V^{IV}$ ,  $Cr^{III}$  or  $Fe^{III}$  or  $Ni^{II}$  as well), iii) rigid coordination modes between the metal centres and ligands (a large coordination number can make it more rigid), iv) ligands with atoms with zero nuclear spin (ligands with Sulphur- donor moiety). Encapsulation of such complexes within host moieties can improve the qubit properties and provide substantial stability. Here we have incorporated different transition metal helicates with encased molecules: i) to realize Multiqubit error correction with one molecule, ii) external manipulation of qubit coherence using light and molecular encapsulation and iii) conditional qubits with  $Ni(II)$  qubits.<sup>3, 4, 5, 6</sup>

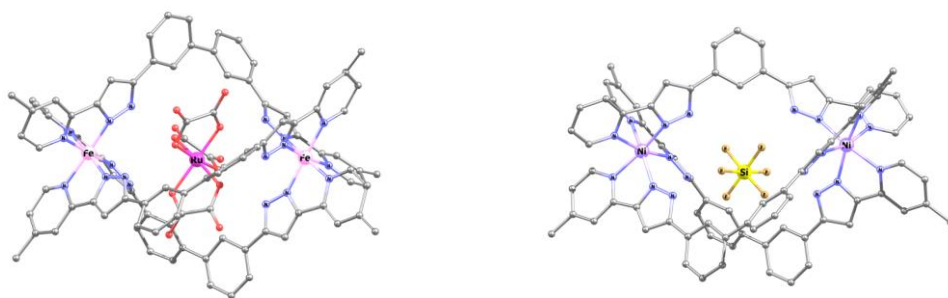


Figure 1. X-ray crystal structure of Ru(III) based qubit encapsulated inside  $Fe_2$  helicates (left) and terminal  $Ni_2$  helical qubits (right).

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## Multifunctionality in Cyanobridged Coordination Networks

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Switchable magnetic materials such as metal to metal electron transfer (MMET) and Spin Crossover (SCO) systems are gaining popularity within the field of coordination chemistry and molecular magnetism owing to their applications in high-density storage and sensing devices, quantum computing, spintronics etc.<sup>1</sup> For application purposes, it is desirable to have ET and SCO materials that are bistable at room temperature and can be tuned by the sight alternation of external stimuli.<sup>2</sup> However, there are few other factors that effect the spintransition/electron transfer phenomenon such as solvent molecules, counter cations/anions, crystal shape and structure etc. To study the magneto structural relationship we have synthesized complexes of different dimensionality using octacyanometalate building blocks  $[M(CN)_8]^{3-}$  (M= Mo, W) and with mono and bidentate ligands with 3d metal centers.<sup>3,4</sup> The detailed magnetic analysis of the synthesized complexes revealed interesting thermo-induced SCO and MMET properties at near room temperature and photo effect under light irradiation at low temperature.

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## Molecular Clusters to Ladders: Designing unprecedented low dimensional Fe-Cu based heterobimetallic cyanometallates.

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Controlled synthesis of supramolecular assemblies with predetermined dimensionality and connectivity has been challenging. While building block approach has been employed to realize various cyanide based heterobimetallic molecular magnets including triangles [Fe<sup>III</sup><sub>2</sub>M<sup>II</sup>], square [Fe<sup>III</sup><sub>2</sub>M<sup>II</sup><sub>2</sub>], trigonal-bipyramids [Fe<sup>III</sup><sub>2</sub>M<sup>II</sup><sub>3</sub>] based molecular magnets where (M = Fe, Mn, Co) with interesting properties, such as single-molecule magnets (SMMs) and single-chain magnets (SCMs), spin crossover (SCO), metal-to-metal electron-transfer (MMET) induced by an external stimuli such as temperature, photoexcitation, and pressure. The incorporation of anisotropic metal centres such as Cu<sup>2+</sup> into molecular magnets has remain unexplored. In this work, we design the novel Fe-Cu- based low dimensional heterobimetallic systems using cyanide-based building block strategy and rationally combine them with multinuclear copper-pyrazole based system as a secondary building unit to understand the effects of dimensionality and establish a magneto structural correlation between the designed systems.

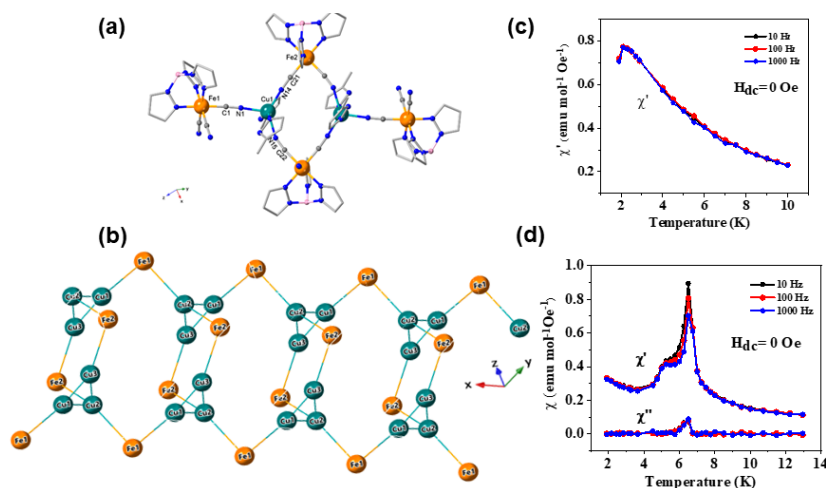


Figure 1: Perspective view of Fe-Cu bimetallic molecular magnets (a) 0D molecular cluster [Fe<sub>4</sub>Cu<sub>2</sub>] (b) 1D ladder [Fe<sub>2</sub>Cu<sub>3</sub>] and their corresponding magnetic properties (c) and (d) respectively.

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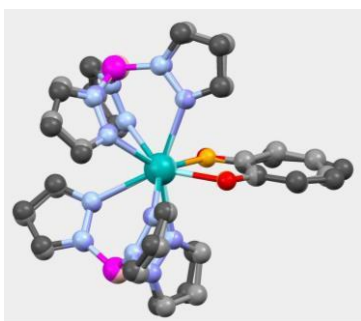


## Exchange coupling and spin parity effects on the magnetization dynamics of Lanthanide-based complexes: an NMR and $\mu$ SR investigation

Lorenzo Sorace<sup>a</sup>

INFN Sez. di Firenze and Department of Chemistry “U.Schiff” University of Florence  
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The research on the effects of exchange-coupling interaction on the spin dynamics of orbitally degenerate lanthanide-based complexes experienced a surge in recent years. On one side, this is due to the advancement in experimental and theoretical approaches. On the other side, lanthanide complexes containing a second spin exchange coupled to the metal center(s) have been reported to display superior properties as single-molecule magnets than those containing the lanthanide as only magnetic center. A disentangling of the effects due to the exchange coupling and to the single ion properties requires both the investigation of a consistent, isostructural set of complexes, and the use of different spectroscopic tools to analyze different timescale regions. Nuclear Magnetic Resonance (NMR) and Muon Spin Relaxation ( $\mu$ SR) emerge in this respect as a set of powerful and versatile techniques which allow a direct investigation of the magnetization dynamics of individual molecules, on a timescale faster than that usually accessible by conventional magnetic techniques such as ac susceptibility. We report here on a combined NMR and  $\mu$ SR investigation of two Terbium(III) and two Dysprosium(III) dioxolene complexes,<sup>1</sup> bound by a diamagnetic (tropolone) or paramagnetic (semiquinone) ligand, all sharing an isostructural first coordination sphere (Figure 1).



**Figure 1**

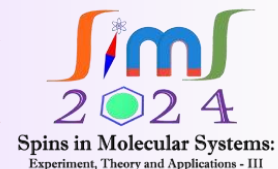
Overlaid structures of Lanthanide-semiquinone (clearer) and Lanthanide-tropolone (darker), evidencing the similarity of their coordination sphere.

The study allowed us to evidence both the role of both the Ln magnetic ions and of the exchange coupling of the radical in determining the spin dynamics of the system; and the complementarity of NMR and ac susceptibility techniques for investigating the spin dynamics in different timescales.<sup>2</sup>

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## Switching in Unconventional Semiconductors

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Mixed semiconductors/conductors with ionic and electronic conductivity are fundamentally interesting due to the intertwining of the DOS which results in electronic transport significantly modified by the ionic defect density. In the first part of the talk we will discuss the demonstration of high performance perovskite transistor. This has been challenging due to the ionic screening of gate modulation. However, with precise chemical control of ionic defect we demonstrate on methylammonium-free, mixed-metal (Pb/Sn) perovskite compositions high mobility reaching  $5.4 \text{ cm}^2/\text{Vs}$ , ON/OFF ratio approaching  $10^4$ , and normalized channel conductance of  $3 \text{ S/m}$ . These results are corroborated with spectroscopic studies.

In the next part of the talk, I will describe another class of metallic bonded organic frameworks. In these materials, we demonstrate that the charge transport is tuned in the channel through a voltage controlled ionic migration. Such facile control of channel conductivity allowed to cleanly demonstrate two distinguishable states of memory with a channel current difference in  $\sim 10^4$ . Moreover, these unique states exhibit memory retention extending to years. Moreover, with suitable device engineering we further demonstrate feature of neuronal learning in these devices. All in all, this opens up niches applications with these class of mixed materials.



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## Speakers for Day 4 : 8<sup>th</sup> November 2024

- 1) Mitsuhiko Maesato
- 2) Michael L. Baker
- 3) Amit Kumar
- 4) Debamalya Banerjee
- 5) Nayanmoni Gogoi
- 6) Magdalena Fitta
- 7) Mathieu Gonidec
- 8) Ramanathan Mahendiran
- 9) Suranjan Shil
- 10) Sreetosh Goswami
- 11) Vamsee Voora
- 12) Fabrice Pointillart
- 13) Indranil Das
- 14) Petr Neugebauer
- 15) Arun K. Bar
- 16) Richard Layfield
- 17) Sergey A. Varganov
- 18) Darshan G Joshi
- 19) Maheswaran Shanmugam
- 20) Arun K. Manna
- 21) Sabyashachi Mishra
- 22) Kalobaran Maiti
- 23) José J. Baldoví
- 24) Federico Totti



## Quantum Spin Liquids

### in Triangular-Lattice Organic Mott Insulators

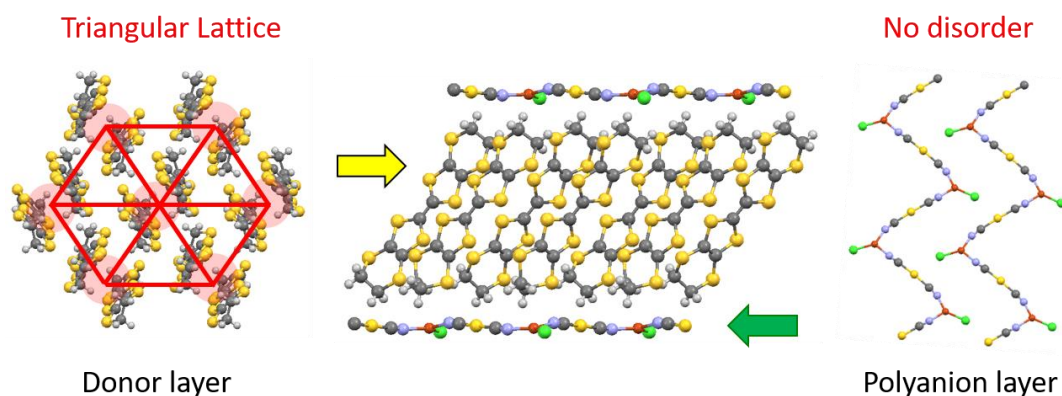
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Quantum spin liquids (QSLs) are exotic states of matter, in which conventional long-range magnetic ordering is suppressed by strong quantum fluctuations. Organic Mott insulators having spin frustrated triangular lattices are good candidates of QSLs.

In 2003, we reported QSL behavior in  $\kappa$ -(ET)<sub>2</sub>Cu<sub>2</sub>(CN)<sub>3</sub> having a nearly regular triangular lattice, where ET denotes bis(ethylenedithio)tetrathiafulvalene [1]. The gapless QSL behavior was also observed in the sister compound  $\kappa$ -(ET)<sub>2</sub>Ag<sub>2</sub>(CN)<sub>3</sub> [2]. On the other hand,  $\kappa$ -(ET)<sub>2</sub>B(CN)<sub>4</sub> with a highly distorted quasi-one-dimensional triangular lattice behaved similarly to QSL, but exhibited a spin-singlet ground state [3].

All organic QSL candidates reported to date have some disorder in their structure, making it difficult to clearly identify the intrinsic nature of QSL. Recently, we have succeeded in obtaining  $\kappa$ -(ET)<sub>2</sub>Cu[Au(CN)<sub>2</sub>]Cl with a disorder-free anion layer (Fig.1) [4] and observed gapless QSL behavior [5]. This compound is a promising material for investigating gapless spinons and the roles of structural disorder and magnetic impurities in QSLs.



**Figure 1** Crystal structure of  $\kappa$ -(ET)<sub>2</sub>Cu[Au(CN)<sub>2</sub>]Cl

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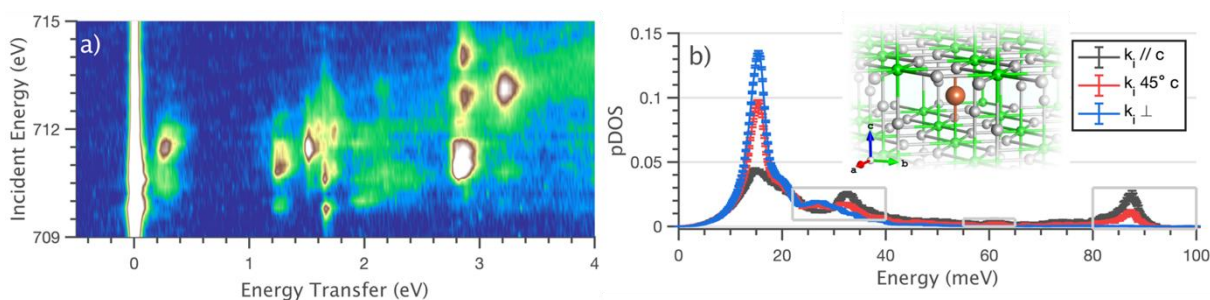
## Quantifying single-ion magnet dynamics with X-ray spectroscopies

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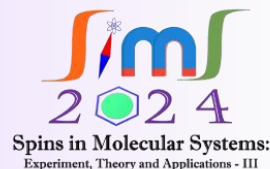
The selection of solid-state compounds with local dopant environments that mimic molecular-based magnets opens up a promising avenue for innovation. This approach allows us to draw from the rich knowledge of molecular magnetism while maintaining a rigid solid-state environment. By doing so we can reduce spin-phonon coupling and uphold rigorous local coordination symmetry. Lithium nitride, in particular, serves as an exemplary extended solid-state host lattice. It can accommodate linearly coordinated transition metal dopants, including Mn(I), Fe(I), Co(I), Ni(I), and Cu(I). Among these, Fe(I) stands out with its exceptional magnetic properties, including a magnetic coercivity field that exceeds many rare-earth-based permanent magnets and an observed magnetic hysteresis of up to 16 K<sup>1</sup>. In this talk, I will delve into the origin of these exceptional properties and underscore the power of X-ray spectroscopies in quantifying local coordination, electronic structure (XAS, RIXS; Figure 1a)<sup>2</sup>, magnetism (XMCD)<sup>3</sup>, and vibronics (NRVS; Figure 1b)<sup>5</sup>. The element selectivity of these methods makes them generally relevant to the study of molecular magnets in non-crystalline environments (including on surfaces) and as a means to access elusive fundamental electronic structure phenomena.



**Figure 1.** (a) Fe L<sub>3</sub>-edge RIXS map of Fe-doped lithium nitride. (b) Single crystal angular-dependent NRVS measurements of Fe-doped lithium nitride yielding the Fe partial density of states. (inlay) Extended solid-state view of Fe-doped in lithium nitride.

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4. submitted for publication.
5. in preparation for publication.



## Understanding of magnetization reversal and its correlations with other physical properties

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The phenomenon of magnetization reversal or negative magnetization (NM) in magnetically ordered systems, where it does not arise due to diamagnetism, is defined as a crossover of dc magnetization from a positive value to a negative value below the magnetic ordering temperature. We have employed neutron diffraction technique to get a microscopic understanding of this peculiar magnetic phenomenon that has been observed in several magnetic systems, such as molecular magnets, spinels, garnets, perovskites, and intermetallic compounds [1-11]. It is also interesting to study the implications of this phenomenon on other physical properties, such as exchange bias (EB) and electrical conductivity. In my talk, I will present some of our recent results in this context. We have obtained a physics understanding of the NM and EB phenomena and their correlations in the negative magnetization materials belonging to perovskites and intermetallic compounds. Particularly, anomalous behavior of EB has been correlated to the temperature/magnetic-field induced spin reorientation phenomenon. Implications of the results on electrical properties will also be discussed to highlight the intercorrelated structural, magnetic, and electrical properties of these materials.

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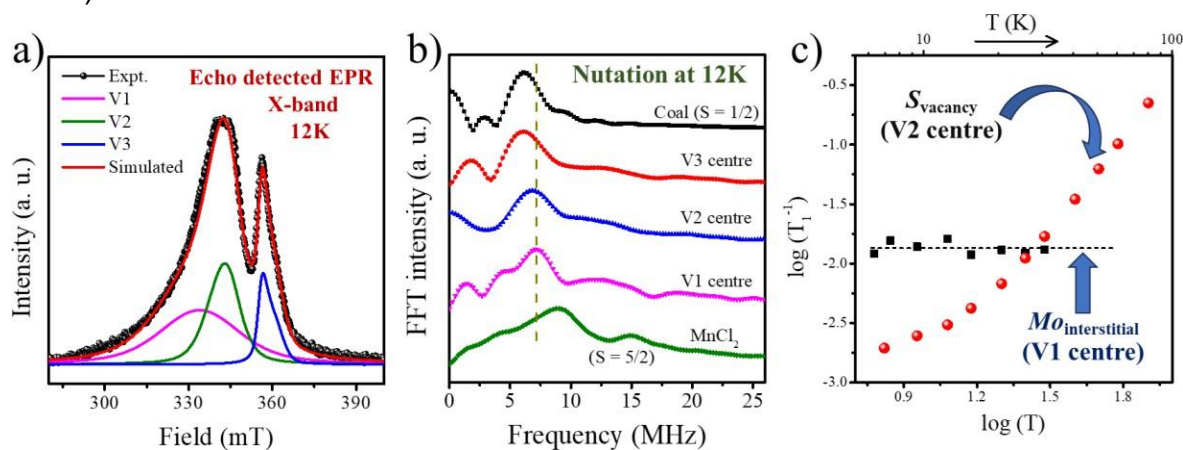
## Exploring Spin Multiplicity in MoS<sub>2</sub>

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The study of native point-defects induced spin centres and synergy of their origin and dynamics are key factors for developing the next generation spintronics and quantum technologies using quasi-2D transition metal dichalcogenides<sup>1</sup>. With the help of low temperature pulsed electron paramagnetic resonance (p-EPR) measurements and first-principles DFT calculations, herein we report for the very first time the presence of high-spin paramagnetic centres Mo<sup>3+</sup> and Mo<sup>2+</sup> in the sulfur deficit hexagonal molybdenum disulfide (2H-MoS<sub>2-x</sub>) nanocrystals. This in-fact opposes the established notion of spin  $S = 1/2$  mediated by the Mo<sup>5+</sup> centres reported so far<sup>2-4</sup>. The intrinsic lattice strain generated in the nanostructure was found to play a crucial role for such spin-localization in this layered material. By performing spin echo measurements, we find that molybdenum interstitial defects ( $S = 3/2$ ) possesses the shortest spin-lattice relaxation time ( $T_1$ ) as compared to the sulfur ( $S = 3/2$ ) and oxygen vacancies ( $S = 1/2$ ). Moreover, the temperature dependent  $T_1$  measurements revealed a direct process for the spin-lattice relaxation of interstitial defects (V1 centre) and a Raman process for the vacancy sites (V2 and V3 centres).



**Figure 1:** (a) Echo detected field swept EPR spectra of MoS<sub>2</sub> nanoparticle at 12 K. EPR lineshape was simulated by considering 3 spin centres, namely V1 (Mo-interstitial), V2 (S- vacancy) and V3 (O-vacancy of MoO<sub>3-x</sub>). (b) Rabi oscillation measurement at the positions of the three spin centres, which were compared with the standard spin-1/2 coal and spin- 5/2 MnCl<sub>2</sub>. Vertical dashed line represents the nutation frequencies of V1 and V2 after Fourier transformation. (c) Temperature dependence of spin-lattice relaxation timescale of V1 and V2 centres. V1 centre is following a direct relaxation process whereas V2 and V3 centres are following Raman process of relaxation.

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## Engineering Water Processable Multifunctional Molecular Magnetic Materials

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Discovery of room temperature magnetism in Prussian blue analogues fevered an outburst of activities to design cyano bridged multifunctional molecular magnetic materials.<sup>1-2</sup> Despite their versatile characteristics, application of such coordination compounds in fabricating functional devices remains a distant goal so far. This can be primarily attributed to the inherent difficulty in post synthetic processing of cyanido bridged coordination polymers owing to their inherent poor solubility. We have recently developed a new approach to access chiral hetero-metallic cyanido bridged coordination polymers which have the unique ability to form stable aqueous colloid without employing any soluble polymer matrix.<sup>3</sup> Decorating cyanido bridged coordination polymer networks with covalently anchored hydrophilic groups remarkably augments their solution processibility. Moreover, the chiral cyanido bridged heterometallic aggregates designed here shows long range ferromagnetic ordering at low temperature, ferroelectric behavior and electric field modulated-EPR signals. Synthesis, structure, magnetic and electric behavior of this new generation of water processable multifunctional cyanido bridged molecular magnetic materials will be discussed during this presentation.

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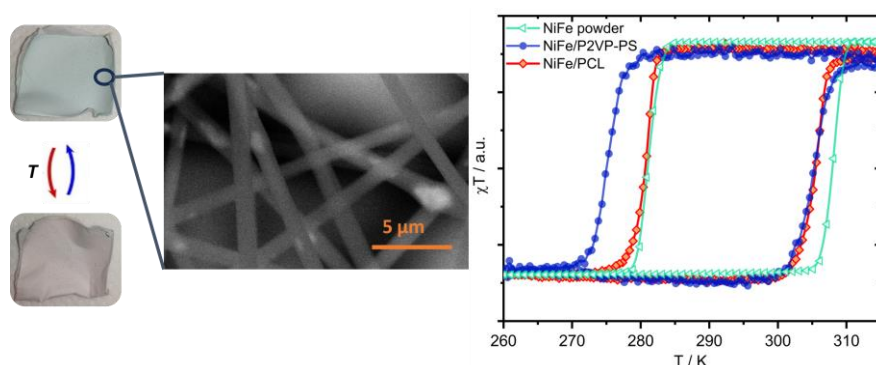
## Stimuli-responsive electrospun composites based on molecular magnets and organic polymers

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One of the most important features of molecular magnets is the ability to switch between two or more well-defined states in response to external stimuli. In coordination systems, this switchability can be achieved through various mechanisms, and the most pronounced effects are observed if the switching process involves conversion between different electronic states of the metal centers, e.g. spin crossover effect or metal-to-metal charge transfer.

This work aimed to incorporate multi-responsive coordination structures into organic polymer matrices to develop composite materials with enhanced versatility and a wider range of applications. To achieve this objective, compounds with varied characteristics were selected and incorporated into poly( $\epsilon$ -lactone) (PCL) and poly(2-vinylpyridine-co-styrene) (P2VP-PS) polymers using the electrospinning technique, resulting in fibrous mesh materials. Additionally, thin foils were fabricated using the drop-casting method to harness the pressure-responsive properties of these robust switchable materials, thereby enhancing the mechanical strength of the composites and expanding their potential applications as molecule-based sensors. Importantly, the switchable properties are maintained in the composite materials, as confirmed by optical observations and magnetic measurements (Fig. 1). Furthermore, the polymer matrix enhances the stability of the compounds under adverse conditions, increasing their usability as sensors for temperature and pressure.



**Figure 1** Left image: Photograph and SEM image of electrospun fibers loaded with  $\{[\text{NH}_4[\text{Ni}(\text{cyclam})][\text{Fe}(\text{CN})_6] \cdot 5\text{H}_2\text{O}]_n\}$ . Right image: Comparison of magnetic susceptibility measurement of loaded electrospun fibers of PCL and P2VP-PS and compound as powder.

## The challenges and rewards of preparing self-assembled monolayers of functional coordination compounds on metallic substrates

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Functional molecular systems could find applications in a broad range of technological systems. To take advantage of the properties of functional molecular systems, over the years, many efforts have focused on grafting a variety of organic molecules and some interesting coordination compounds comprising ad-hoc modifications to allow to bind them specifically to a substrate of choice for the envisioned application. Most often, this is done by using sulfur based anchoring groups on coinage metals or alternate anchoring groups (phosphonic acids, carboxylic acids...) on metal oxides. Our groups focus on the design and study of functional coordination compounds for a wide range of applications going from molecular electronics and spintronics to quantum computing. Coordination compounds are highly versatile systems that present multiple options for tuning their electronic structure and thus their physical properties making them targets of choice for physical-organic studies on surfaces. In this presentation, we will outline the work that we have performed in recent years to successfully graft a variety of switchable Fe (II) Spin crossover (SCO) complexes that retain their properties on metallic surfaces and are highly interesting systems for molecular spintronics. We will also outline recent efforts to anchor chiral Ru paddlewheel coordination complexes on surfaces for the study of the CISS effect in large-area molecular junctions, and will present some recent work on the grafting of Gd-based qubits.



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## Giant magnetostriction in perovskite oxides

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Magnetostriction (MST) refers to the magnetic field-induced strain in a material and it arises from coupling between spin and lattice through orbital degree of freedom. It is quantified through the fractional change in the length ( $\Delta L/L = [D(H) - D(H=0)]/D(H=0)$ ) of a sample subjected to a magnetic field ( $H$ ). Although transition metal oxides (TMO) exhibit an order of magnitude smaller MST than rare earth-based metallic alloys such as Terfenol-D, mechanical, and chemical stabilities together with low-cost of synthesis make TMO attractive for certain applications. So far, oxides with spinel structure have been explored extensively for MST. Among the spinel oxides,  $\text{Co}_2\text{FeO}_4$  shows the highest MST ( $100\text{--}400 \times 10^{-6}$ ) at room temperature and it arises from strong spin-orbit interaction of  $\text{Co}^{2+}$  ( $d^7$ ) ion. Most perovskite oxides show much smaller MST ( $< 60 \times 10^{-6}$ ) even at 10 K. Recently, a giant MST of  $1000\text{--}3000 \times 10^{-6}$  has been discovered in some Mn and Co based perovskite oxides. Such a high value of MST requires different explanations than the conventional mechanism proposed for rare earth alloys. In this talk, I will give an overview of giant MST in perovskite oxides, mechanisms involved, and scopes for enhancing the value of MST. I will conclude with an overview of MST in spin crossover molecular complexes.

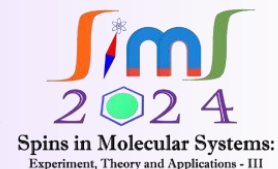
Acknowledgements: R. M acknowledges the Ministry of Education, Singapore for supporting this work (Grant number: A-8000924-00-00 & A-8001933-00-00)

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## Effect of orbital manipulation to tune the magnetic interaction in organic diradicals

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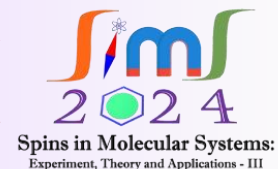
High spin organic radicals are extensively studied experimentally as well as theoretically to get the strong stable organic magnet. However, getting a strong organic magnet is still challenging due to the small intramolecular magnetic interactions in organic systems. By understanding the mechanism of magnetic interaction in organic molecules we can design new strong organic magnetic molecules. Although the mechanism is somewhat known as itinerant exchange, however, this mechanism could not explain the strength of magnetic interaction. To address this issue, we have studied the magnetic interactions in several organic diradicals to understand the mechanism and try to design new molecules with strong intramolecular magnetic coupling. In the earlier work, it has been shown that the magnetic interaction between two spin centers occurs via interaction between singly occupied molecular orbitals (SOMOs), however, various authors claim that this gap varies from molecule to molecule and there is no uniformity. We have concentrated on the gap between the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), namely HOMO-LUMO gap. Surprisingly, we have found that the HOMO-LUMO gap is the key factor for the strength of magnetic interaction in the organic systems where itinerant exchange is predominant. We provided a new mechanism of magnetic interaction where the interaction occurs between two SOMOs via LUMO. Our findings highlighted the importance of HOMO and LUMO for the magnetic interactions, along with the position and orientations between the molecular orbitals.

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## Molecular Neuromorphic Building Blocks for Artificial Intelligence

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Molecular electronic switches have been a research topic for about three decades. The first wave in the nineties revolved around the appealing concept that molecules might make controllable nano-scale switches by self-assembly. However, the molecules proved to be fragile, and their switching endurance was far too low to be useful. Recently, molecular memristive circuit elements based on redox-active transition metal complexes of azo aromatic ligands have demonstrated resistive switching performance superior to inorganic oxides, which calls for a serious examination of their chemical and physical properties and potential applications. Beyond being a simple on-off switch or binary storage element, molecular memristors offer several unique features: deterministic (as opposed to stochastic) and uniform (as opposed to filamentary) resistance switching, multiple resistance levels, simultaneous memristance and memcapacitance, and multiple serial non-monotonic switching events. Can these characteristics offer a significant benefit to computing performance? In this presentation, I will introduce a new generation of molecular circuit elements designed to capture intricate, reconfigurable, dynamic logic within nano-scale material properties. These devices, teetering on the edge of instability, hold promise for emulating brain functions. Our exploration spans from fundamental device principles to the investigation of circuits and on-chip integration [1-7] 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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# Polarization Induced Quantum Confinement of Negative Charge Carriers by Organic Nanoporous Frameworks

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Organic electronics face performance limitations due to low charge carrier mobilities which has stymied their broader applicability. This limitation can be partly attributed to weak intermolecular electron-transfer coupling between the orbitals of neighboring molecules due to their localized nature. Using recently developed single-pole polarization models, in this talk, we discuss an unconventional electron transport pathway for nanoporous frameworks, consisting of diffuse electronic states that are localized within the interior of nanopores or away from the molecular scaffold. These “nanopore states” bound by long-range polarization forces, exhibit distinct features compared to conventional transport pathways, while exhibiting enhanced electronic coupling. The difference between the nanopore-states and quantum corral type states is elucidated. This suggested new pathway, if accessed even transiently, could pave the way for improved properties of organic electronics based on nanoporous frameworks.

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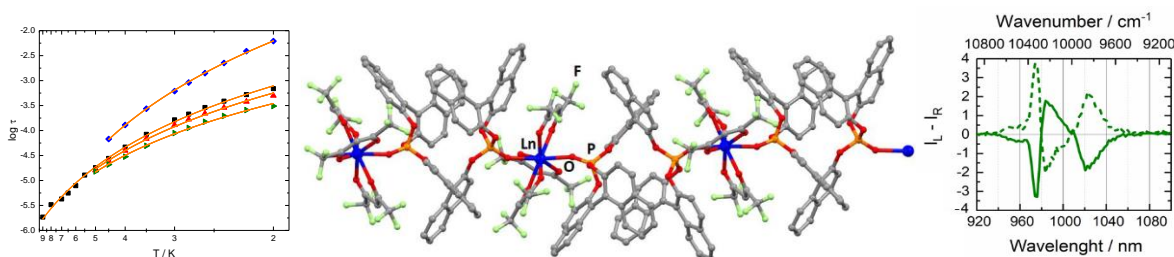
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## Circularly Polarized Luminescence in Single-Molecule Magnets

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Molecular magnetism is a fascinating and more than ever active research field. Substantially a molecular magnet behaves at low temperature like a tiny magnet. Lanthanides, thanks to their peculiar electronic structure, play a central role in preparation of this kind of compounds. In addition, coordination of appropriate chiral ligands to these metals, that are also known for their characteristic luminescent properties, lets to prepare compounds potentially able to emit left and right circularly polarized light with different intensities, a phenomenon called circular polarized luminescence (CPL).<sup>(1)</sup> In this context, the possibility of coexistence of molecular magnetism and chiroptical properties is really attractive. In the present communication, the use of a series of highly optical active binaphthyl derivatives are proposed for the design of coordination complexes involving lanthanide ions. The family of binaphthyl ligands allows the coordination of lanthanides for the observation of Circularly Polarized Luminescence (CPL) and/or Single-Molecular Magnet (SMM) behavior in both solution and solid-state leading to the design of unprecedented 1D assembly of NIR CPL SMM for Yb(III) analogue.<sup>(2)</sup> Recent results about using helicene ligands in lanthanide coordination systems for CPL<sup>(3)</sup> and the possibility to measure CPL spectra at low temperature (4 K)<sup>(4)</sup> will be exposed.



**Figure 1** (Left) thermal variation of the magnetic relaxation time, (middle) X-ray structure of binaphthyl-based Yb<sup>III</sup> polymer and (right) NIR CPL in solid-state.

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# Synergy of Electronic Band Topology and Non-Trivial Magnetism

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The realization of non-centrosymmetric magnetic Weyl metals is anticipated to yield unique anomalous transport properties arising from the interplay between bulk electronic topology and complex magnetic structures. In this talk, we present the discovery of a rare spin-valve-like magnetoresistance at room temperature in the bulk ferromagnetic Weyl metal  $\text{Mn}_2\text{PdSn}$ , which crystallizes in the inverse Heusler (iHA) structure. This system exhibits a substantial anomalous Hall conductivity (AHC) mediated by intrinsic Weyl nodes. A simple substitution of tin with indium leads to the emergence of a double-spin-glassy transition, though the origin of the AHC remains unchanged. Further chemical tuning, achieved by replacing half of the palladium atoms with Iridium to form  $\text{Mn}_2\text{Pd}_{0.5}\text{Ir}_{0.5}\text{Sn}$  in a tetragonal  $D_{2d}$  structure, introduces the conditions required for the stabilization of an anti-skyrmion phase. This transformation results in a giant topological Hall effect, alongside the presence of 42 Weyl node pairs near the Fermi surface, contributing to a significant intrinsic AHC. The talk will conclude with a discussion on the simultaneous realization of topological electronic band structures with magnetic phases in correlated polar magnets and investigation of critical behavior employing AHC, highlighting the potential to leverage novel quantum functionalities.

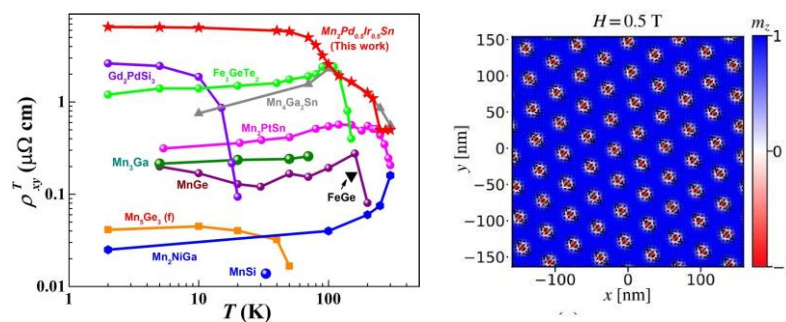


Figure 1: (a) Comparing the topological Hall effect of  $\text{Mn}_2\text{Pd}_{0.5}\text{Ir}_{0.5}\text{Sn}$  with other known topological magnetic materials. (b) Simulated anti-skyrmion image using experimental inputs

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2. Critical behavior and phase diagram of skyrmion-hosting material  $\text{Co}_3.6\text{Fe}_4.4\text{Zn}_8\text{Mn}_4$  probed by anomalous Hall effect. - *Ahmed et al. J Alloys Comps 960, 170274 (2024)*



## Rapid scan ESR: A Versatile Tool for the Spin Relaxation Studies at (sub)THz Frequencies

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The development of pulse electron spin resonance spectroscopy at microwave frequencies above 100 GHz is rather challenging and expensive task due to the low output power of modern high-frequency solid-state electronics. However, there is a number of scientific problems, e.g., DNP enhancement of NMR, that require spin relaxation measurements at THz frequencies. The rapid scan ESR is an alternative technique that does not require high microwave power and still provides information on the spin relaxation times. The method takes advantage of fast sweeps of the excitation microwave frequency over the ESR line. When the frequency sweep reaches a sufficiently high rate, distinct oscillations (also called wiggles) appear in the spectrum<sup>1-3</sup>. It is possible to retrieve the undistorted (slow-scan) spectrum by employing the Fourier Transform analysis as Josef Dadok had demonstrated in NMR<sup>4</sup>. On the other hand, these oscillations bear information about the electron spin-spin relaxation time, which can be extracted via fitting the rapid scan spectrum using the modified Bloch equations. This technique allows one to capture the spin-spin relaxation time at the nanosecond time scale. Furthermore, the particular design of modern high-frequency ESR spectrometers greatly facilitates the multifrequency operation bringing the spin relaxation measurements to an unprecedentedly broad range of magnetic fields using only one ESR spectrometer (Fig. 1). Finally, we will discuss the future steps necessary to make the THz rapid scan ESR a convenient and easy to use tool for the broad scientific community.

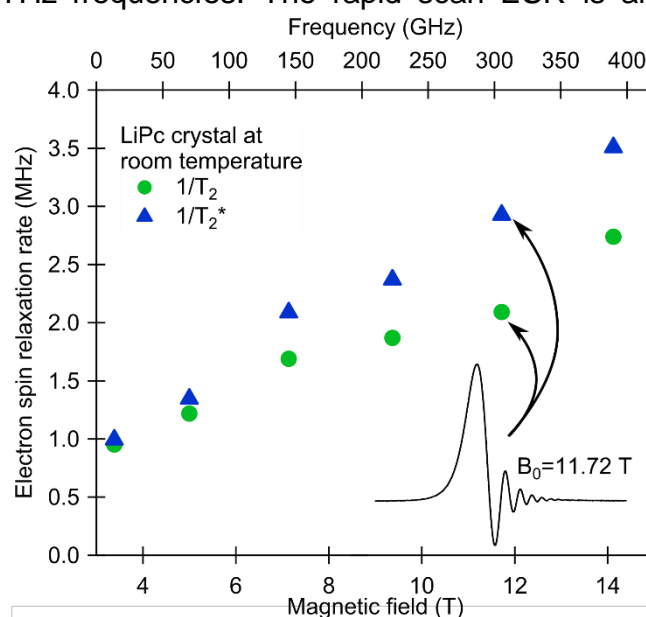


Fig.1 Magnetic field dependence of the electron spin relaxation times  $T_2$  and  $T_2^*$  in LiPc at room temperature.

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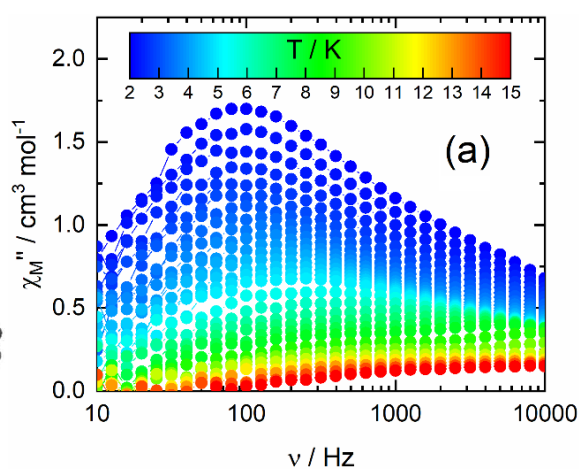
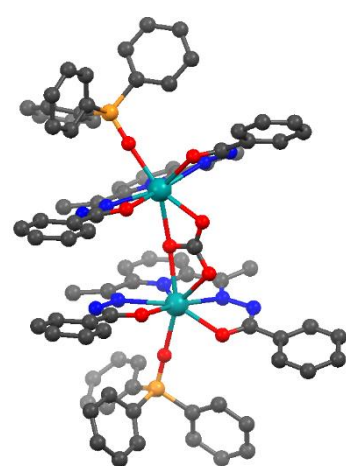
## CO<sub>2</sub> gas as a resource for deriving lanthanide(III) magnetic motifs: tailoring SMM behavior *via* post-synthetic inner coordination modification

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Lanthanide (Ln) ions, especially the Dy(III), exhibit fascinating SMM behaviour.<sup>1</sup> On the other hand, one of the scariest concerns in the modern era is the excessive increment of greenhouse gas CO<sub>2</sub> in



**Figure 1** *Left:* The single-crystal X-ray molecular structure of the dinuclear Dy(III) analogue incorporating triphenylphosphine oxide at the terminally axial coordination sites. Color code: cyan, Dy; orange, P; red, O; blue, N; and grey, C. The H atoms are omitted for clarity. *Right:* The *out-of-phase* ac susceptibility of the magnetization of the Dy(III) analogue under zero applied magnetic field.

the atmosphere. It has already brought forth potential threat to the human civilization.<sup>2</sup> Herein will be presented a facile chemical route to convert CO<sub>2</sub> gas into CO<sub>3</sub><sup>2-</sup> and concomitant formation of a novel series of CO<sub>3</sub><sup>2-</sup>-bridged dinuclear Ln(III) complexes (Figure 1). The dinuclear Ln(III) complexes are found to provide the feasibility of inner coordination post-synthetic modification. The presentation will also be extended to how the slow relaxation of the magnetization of

the Dy(III) analogues can be remarkably tailored by tuning the ligand at the terminally axial coordination sites. For example, the Dy(III) analogue with MeOH at the terminally axial coordination sites exhibit field-induced single-molecule magnet (SMM) behaviour. It renders zero-field SMM behaviour upon substituting the coordinated MeOH with triphenylphosphine oxide.

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## Organometallic Approaches to Lanthanide SMMs

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Synthetic coordination chemistry is a driving force in the development of molecular magnetism. Studies of single-molecule magnets (SMMs) have incorporated a bewildering variety of ligands over the last 30 years, most of which lie in the realms of classical coordination chemistry.<sup>1</sup>

Our group introduced organometallic synthesis as a method for the design and synthesis of lanthanide SMMs,<sup>2</sup> an approach that has since grown in popularity. Many types of carbon-donor ligand are now used to address the main SMM performance parameters, with cyclopentadienyl (Cp) ligands proving to be popular in the large and growing family of organometallic lanthanide SMMs.<sup>3</sup> The organometallic approach to lanthanide SMMs also gives access to soft ligands based on heavier p-block elements, introducing possibilities for targeting the crystal field through enhanced covalency in the metal-ligand bonding.<sup>4</sup>

In this lecture, our recent work on a series of SMMs containing hetero-Cp ligands with additional germanium and tin donor atoms will be presented, highlighting unusual ligand non-innocence effects and their impact on the magnetism.<sup>5</sup> In addition, a new synthetic approach in which the reactivity of 'masked' divalent lanthanides is used to access SMMs containing lanthanides in the trivalent oxidation state will also be introduced.<sup>6</sup>

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## Nonadiabatic molecular dynamics with the crystal field Hamiltonian to study spin dynamics in lanthanide complexes

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Understanding the spin dynamics in paramagnetic lanthanide complexes is critical for developing molecular magnets and qubits with high blocking temperatures and long spin relaxation times.<sup>1,2</sup> Because of the size and complexity of the electronic structure of metal complexes, most theoretical and computational efforts aimed at understanding their spin dynamics utilize different statistical methods. While these methods can predict experimentally measured quantities, the complete picture of spin dynamics, which is important for designing molecular magnets and qubits with desired properties, is often missing. We developed a new computational methodology based on the nonadiabatic molecular dynamics<sup>3</sup> and the crystal field theory to simulate the spin relaxation in paramagnetic lanthanide complexes. This development includes 1) implementing the energy gradient and nonadiabatic (spin-vibrational) coupling for the crystal field theory,<sup>4</sup> and 2) interfacing the crystal field theory with the *ab initio* multiple spawning (AIMS) molecular dynamics.<sup>5</sup> The new nonadiabatic molecular dynamics provides unprecedented insight into the vibration-mediated transitions between different spin states of lanthanide complexes.

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## Topological excitations in quantum magnets

Darshan Joshi

Magnetic excitations such as magnons or triplons can have non-trivial topology associated with them. Consequently, these systems may host topologically protected end-state excitations, which could potentially be used for spintronics applications. In this talk, I will demonstrate that a simple model system of spin-1/2 on a 1d ladder can host topological excitations leading to protected fractionalized end states. Such ladder systems can be found in many quantum materials. We show that using an external magnetic field we can switch between a topological and trivial phase. We also demonstrate a way to detect these end excitations directly. Further, we will discuss how similar topological magnets are possible in 2d materials.



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**MODERN TRENDS IN MOLECULAR MAGNETISM – IV**  
**&**  
**SPINS IN MOLECULAR SYSTEMS:**  
**EXPERIMENT, THEORY AND APPLICATIONS – III**



**Maheswaran Shanmugam**



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# Computational Design of Metal-Free Functional Organic Molecules for Efficient Triplet Photosensitization

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Large excited singlet-triplet gap and small spin-orbit coupling in heavy-metal free organic molecules limit the intersystem crossing (ISC) and thereby, the triplet photosensitization efficiency. Molecular-twist and/or heteroatom substituents were shown to promote the ISC in several organic molecular systems.<sup>1</sup> Time-dependent density functional theory based computational modelling studies can provide a detailed understanding on the role of molecular-twist and/ or heteroatom substituents in tailoring ISC, which greatly helps designing efficient triplet photosensitizers. But, computational results, in particular excited-state energies and SOC are often highly dependent on the choice of density functional. Non-empirically and optimally tuned range-separated hybrid has been proven to produce a reliable and quantitatively accurate description of the excited-state electronic structures including SOC.<sup>2,3</sup>

In this talk, I shall present and discuss some of our recent modelling studies on the triplet photosensitization in a few chalcogen-substituted  $\pi$ -conjugated organic molecules. More specifically, the excited-state electronic structures including the SOC are obtained from time-dependent optimally-tuned range-separated hybrid along with the ISC rates from Fermi-golden rule.<sup>3-9</sup> Quantitatively accurate energies of the electronically excited singlets and triplets combined with appropriate theoretical protocols are shown to yield a reliable and predictive description of the ISC. Importantly, ISC efficiency is predicted to substantially enhance through molecularly engineered chalcogen substituents in the studied molecules.<sup>4-9</sup>

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## Quantum Chemistry on a Quantum Device:

### Algorithm and Application

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Quantum computers have the potential to revolutionise the field of quantum chemistry by exploiting the principles of quantum mechanics to perform complex calculations with unprecedented speed and accuracy. The current era of quantum computers works with a limited number of qubits and inherent noise. Variational quantum algorithms (VQAs) are currently the best tools for working within these constraints. The VQAs use a classical optimiser to train a parametrised quantum circuit. For molecular applications, there are several classical optimisers available. We recently employed VQA to estimate molecular properties (e.g., the ground state energy, dissociation energy, and dipole moment) of systems described with 2 to 10 qubits. Our study provided a detailed comparative account of the performance of various classical optimisers and classified them based on their efficiency and noise resistance [1]. The benchmarked methods are also applicable in other classes of problems [2]. However, even the most efficient classical optimiser suffers from inherent noise that increases with system size. To address this issue, we have recently proposed a scheme within which a partial (qubit) Hamiltonian is solved by selecting a limited number of terms of the qubit Hamiltonian. The partial Hamiltonian, constructed with fewer Pauli strings, estimates the energy at a much lower computational cost and diminished noise. This approach has been demonstrated as an initialisation technique for complex systems [3].

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## Anomalies and Kink in topological Kondo lattice systems

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Topological insulators are simple bulk insulators with symmetry protected metallic surface states which exhibit Dirac cone like dispersions. Most of the topological systems studied are weakly correlated. The properties of these massless Dirac fermions in the presence of electron correlation is an interesting emerging area of research where electron correlation is expected to enhance the effective mass of the particles. We studied the behavior of Dirac fermions in novel Kondo lattice system employing ARPES. We find that a binary system, SmBi show signature of multiple gapped and un-gapped Dirac cones in the band structure [1,2]. Employing ultra-high-resolution ARPES, we discover destruction of a surface Fermi surface across the Neel temperature while the behavior of Dirac cones survives across the magnetic transition. HAXPES data of a non-symmorphic Kondo lattice system, CeAgSb<sub>2</sub> and CeCuSb<sub>2</sub> exhibit unusual behavior; despite bulk properties show Kondo behavior, the typical Kondo feature is not observed. Instead, we find a new feature in the core level spectra [3,4]. The ARPES data of CeAgSb<sub>2</sub> show distinct Dirac cones as well as diamond-shaped nodal lines; the slope of these linear bands is unusually high, larger than that in graphene and maintains its high value in a wide energy range indicating robust high velocity of these relativistic particles [5]. The slope becomes smaller in the vicinity of strongly correlated Ce 4f bands forming a kink; a unique case due to correlation induced effects.

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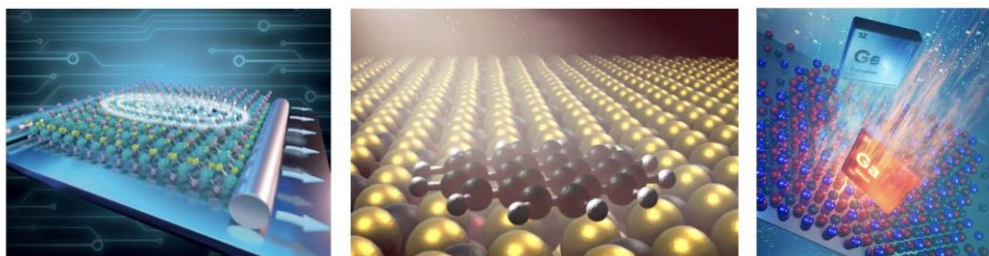
## Engineering 2D magnetism in van der Waals materials using first principles

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The recent isolation of two-dimensional (2D) magnets offers tantalizing opportunities for spintronics, magnonics and quantum technologies at the limit of miniaturization. [1] Among the key advantages of atomically-thin materials are their flexibility, which provides an exciting avenue to control their properties by strain engineering, and the more efficient tuning of their properties with respect to their bulk counterparts.

In this presentation, I will provide an overview of our recent results on this fascinating topic. First, we will take advantage of the outstanding deformation capacity of 2D materials to answer the question: Can we use strain engineering to control spin waves propagation? [2] For that, we will focus on the magnetic properties, magnon dispersion and spin dynamics of the air-stable 2D magnetic semiconductor CrSBr, investigating their evolution under mechanical strain and Coulomb screening using first-principles. Then, we will introduce the modulation of the magnetic properties, magnon dispersion and spin dynamics of this 2D magnet after the deposition of sublimable organic molecules in a journey towards molecular controlled magnonics. [3] On the other hand, we will look for topological magnons in chromium trihalides ( $\text{CrX}_3$ ), [4] investigate magnetostriction effects in 2D van der Waals antiferromagnets such as  $\text{FePS}_3$  and  $\text{CoPS}_3$ , [5] create new Janus 2D magnetic materials based in  $\text{MPS}_3$  in order to answer: what are the effects of mirror broken symmetry on the magnetic properties? [6], and finally, we will delve into the origin of above-room-temperature magnetism in  $\text{Fe}_3\text{GaTe}_2$  [7].



**Figure 1:** Artistic representation of (left) magnon straintronics device showing the chemical structure of CrSBr; (center) an irradiated coronene molecule on the surface of a 2D magnetic material; (right) formation of a  $\text{Fe}_3\text{GaTe}_2$  single-layer representing the enhancement of TC with respect to  $\text{Fe}_3\text{GeTe}_2$ .

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## Elective Affinities: when Molecular Magnets Meet the Surface

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The progression towards devices based on Molecular Magnets involves several crucial steps, with adsorption on the surface (@surface) being the initial and most critical one. Traditionally, the design of hybrid systems (MM@surface) aimed to "rigidly" transfer the bulk properties of Molecular Magnets directly onto the surface. Recently, however, a new paradigm has emerged: leveraging new 2D properties and making the surface an active player. The computational characterization of these systems has played a pivotal role, first by rationalizing and then guiding the experiments. This talk will present key cases where elective affinities have played varying roles<sup>1,2,3,4</sup> in the development of these systems.



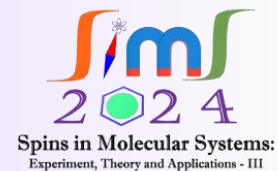
Figure 1 Main characters

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MODERN TRENDS IN MOLECULAR MAGNETISM – IV  
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# POSTER PRESENTATIONS



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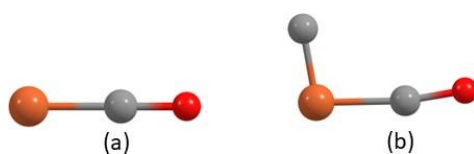
# Magnetic and Electronic Properties of FeCO and FeC<sub>2</sub>O Molecules: A Computational Study

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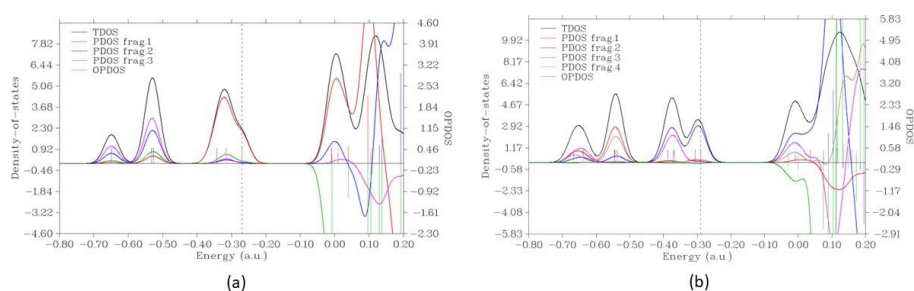
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The present study attempts to study the magnetic properties of FeCO and FeC<sub>2</sub>O molecules using advanced computational methods, such as density functional theory (DFT) and multi-reference ab initio methods. Iron-based compounds are notably significant in single-molecule magnet (SMM) research as iron has many spin states and can undertake potent magnetic interactions when joined with pertinent ligands. With iron and potent field ligands, the FeCO and FeC<sub>2</sub>O molecules show a fascinating possibility for SMM features due to the possible interaction between the metal center and ligand. DFT with hybrid functionals are utilized to optimize geometries (shown below) and examine the spin density distribution. The density of states plot is also shown below. The magnetic anisotropy of the molecules is obtained using ab-initio methods, and spin-orbit coupling is studied to determine whether the molecules can sustain magnetic memory at low temperatures, an essential attribute of SMMs. This study probes the electrical and magnetic properties of FeCO and FeC<sub>2</sub>O molecules, providing insights into their potential as single-molecule magnets and improving the understanding of magnetic characteristics in transition metal carbonyl complexes. The findings complement the apprehension of magnetism in transition metal-oxalate complexes, establishing a foundation for realizing new SMM candidates. Further experimental studies are necessary to confirm the SMM properties of FeCO and FeC<sub>2</sub>O molecules and explore their potential applications.



**Figure 1:** Optimized geometries of (a) FeCO and (b) FeC<sub>2</sub>O.



**Figure 2:** The density of states plot of (a) FeCO and (b) FeC<sub>2</sub>O

**Keywords:** Single-molecule magnets; magnetic anisotropy; spin-orbit coupling; spin density distribution; transition metal carbonyl complexes; transition metal-oxalate complexes.

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MODERN TRENDS IN MOLECULAR MAGNETISM – IV  
&  
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EXPERIMENT, THEORY AND APPLICATIONS – III



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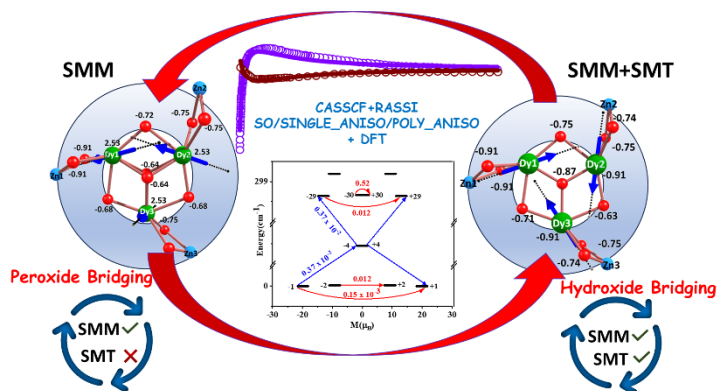
## Single-molecule magnetic and Single-molecule toroic behavior of 3d-4f complexes.

Amit Gharu<sup>a</sup> and Kuduva R. Vignesh<sup>a\*</sup>

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Single molecular magnets (SMM<sub>s</sub>) are the molecules that show magnetic relaxation below their blocking temperature ( $T_B$ ) in the absence of the magnetic field. SMMs are highly interesting due to their potential application in memory storage devices, Q-bits, etc.<sup>[1]</sup> SMMs were primarily searched on the 3d or Lanthanide (Ln) based mononuclear and polynuclear complexes. Due to the combination of the large spin of 3d ions and the spin/anisotropy of lanthanide ions, heterometallic 3d/4f complexes have recently attracted much attention. Moreover, some polynuclear 4f/3d-4f systems show Single-molecule toroics (SMTs) behavior which are bistable molecules similar to single-molecule magnets (SMMs) but with a toroidal magnetic state. The noncollinear arrangement of the magnetic moments of each metal center in SMTs can lead to interesting magnetic properties due to their high molecular symmetry.<sup>[2]</sup> Here, we discuss the magnetic behavior of a series of  $\{M^{III}_3Ln^{III}_3\}$  ( $M = Ni, Zn$  and  $Ln = Dy, Tb, Gd$ ) complexes.<sup>[3]</sup> Ab initio and Density Functional Theory (DFT) calculations were performed using MOLCAS 8.2 and GAUSSIAN 16 programs, respectively and the calculations align with the experimental prediction. Structural parameters and computational studies for the  $\{Co^{III}_4Ln^{III}_2\}$  ( $Ln = Tb, Dy, Ho$ ) system will also be discussed.



**Figure 1.** The role of bridging ligands in modulating 3d-4f SMM and SMT Behavior.

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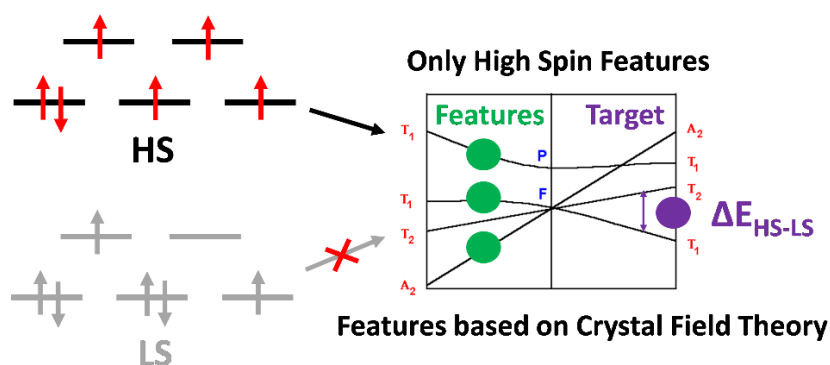
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# Unlocking simple features to predict DFT spin state gaps of 3d metal complexes using Machine Learning

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Determining accurate spin state gap energies (SSE) in 3d transition metal complexes (TMC) is a longstanding challenge in theoretical chemistry. Discrepancies arise from the disparate treatment of high spin (HS) and low spin (LS) structures by electronic structure methods, owing to their varying electron correlation<sup>1</sup>. Addressing this disparity, we propose employing machine learning (ML) algorithms trained on features derived from cost-effective DFT calculations solely for HS states to predict SSE values, thereby circumventing the need for computationally intensive LS calculations. Notably, DFT calculations for HS cases have lower convergence issues and are more reliable due to their lower multireference character<sup>1</sup>.



**Figure 1** Schematic representation of this work

Feature vectors encompass straightforward properties derived including valence MO eigenvalues, MO coefficients of d-orbitals, NPA charges, and basic structural information of the complexes. Interestingly, incorporating experimental atomic spectra<sup>2</sup> levels of bare metal ions enhances SSE prediction accuracy, achieving an impressive R<sup>2</sup> score of 0.90 and minimal mean absolute error (MAE) of 3.8 kcal/mol for SSE predictions. The model based on Werner type complexes demonstrated transferability to complex π based systems.

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## Post-synthetic miniaturization of multifunctional chiral cyanido-bridged Mn(II)-Fe(III)/W(V) network

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Constructing nanoscale devices using magnetic materials enriched with multifunctionality has emerged as one of the most compelling challenges in recent times.<sup>1</sup> In this regard, considerable research interest has been focused to the development of molecular magnets decorated with a range of intertwined characteristics e.g. magnetochiral dichroism (MChD), multiferroicity, guest or light responsive magnetism, magnetocaloric effect, conductivity, etc.<sup>1</sup> However, despite their versatile characteristics, examples of such coordination compounds exhibiting multiferroic behaviour are relatively scarce and application of such compounds in fabricating functional devices remains a distant goal so far.<sup>2</sup> The former can be primarily attributed to the fact that chirality must be controlled in the molecular structure as well as in the entire crystal structure while the later refers to the inherent difficulty in post synthetic processing of cyanido bridged coordination polymers owing to their inherent poor solubility. We have recently developed a new approach to access chiral heterometallic cyanido bridged coordination polymers which have the unique ability to form stable aqueous colloid without employing any soluble polymer matrix.<sup>3</sup> Decorating cyanido bridged coordination polymer networks with covalently anchored hydrophilic groups remarkably augments their solution processibility. Moreover, the chiral cyanido bridged heterometallic aggregates designed here shows ferrimagnetic ordering and electric hysteresis loop. Synthesis, structure, magnetic and electric behaviour of this new generation of water processable multifunctional cyanido bridged Mn(II)-Fe(III)/W(V) molecular magnetic materials will be discussed during this presentation.

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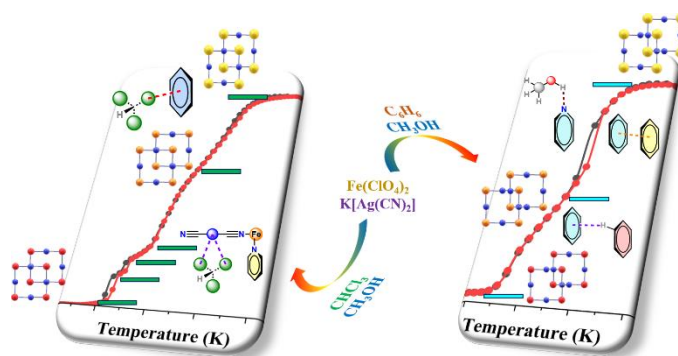
# Interplay of lattice cooperativity and elastic frustration influencing SCO behaviour in two Fe<sup>II</sup>-[Ag(CN)<sub>2</sub>] Hofmann CPs with distinct interpenetrated structures

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Hofmann-type coordination polymers (CPs) exhibit interesting spin crossover (SCO) profiles ranging from a single-step to an abrupt, hysteretic, and multi-step transition.<sup>1,2,3,4,5</sup> Their porous nature enables the incorporation of various guests that modulate the nature of the non-covalent interactions, directly affecting the SCO profile.<sup>2,3,4,5,6</sup> Such interactions between host and guests can induce symmetry breaking in the structure, thereby giving rise to multistep transitions.<sup>1,3,4</sup> Recent studies focus on introducing structural features that can induce elastic frustration and symmetry breaking, stabilizing different intermediate spin-states. The dicyanoargentate [Ag(CN)<sub>2</sub>]<sup>-</sup> units usually form interpenetrated networks, stabilized by argentophilic interactions, accompanied by other non-covalent interactions. Herein, we tuned the interpenetration in two double-layered dicyanoargentate Fe<sup>II</sup>-Hofmann CPs and manipulated the cooperative interactions between the successive layers of the CPs. Overall, the elastic frustration outweighed the lattice cooperativity resulting in multi-step SCO in both the CPs. The rotation of the pillar ligand (DPyN) modulated the non-covalent interactions with the crystallized solvent and accommodated the structural reorganization associated with SCO in the CPs. Such studies provide a better understanding of the interplay of lattice cooperativity and elastic frustration in determining the SCO behavior in CPs.



**Figure 1** Schematic representation of the SCO profiles of the CPs.

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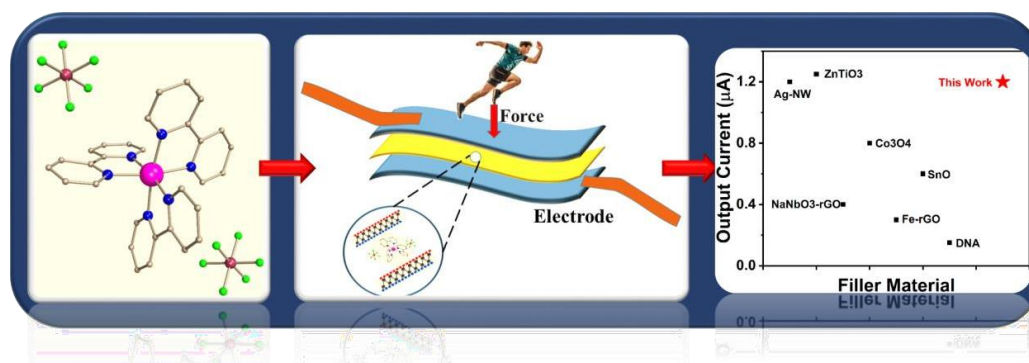
## A Molecular Based Piezoelectric Nanogenerator for Sustainable Energy Harvesting using a ferroelectric Co(II) complex

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Energy harvesting offers a sustainable power source, enabling long-term self-powered nanodevices. We focused on flexible polymer-based piezoelectric nanogenerators, particularly using PVDF, due to its flexibility, cost-effectiveness, and ability to harvest energy from various environmental sources like vibration, mechanical load, human motion and waste heat. However, PVDF's practical use is limited by its low piezoelectric response, which depends on the proportion of the polar  $\beta$ -phase. To overcome this, we synthesized a Co(II) complex with a bipyridine ligand, which crystallizes in the polar P31 space group. Integrating this complex into a PVDF matrix significantly increased the  $\beta$ -phase content from 10.4% to 60.2%, as confirmed by FTIR. A composite film with 10 wt% of the complex achieved an 13.5 V peak-to-peak output, a power density of  $1.21 \mu\text{W cm}^{-2}$ , and a current of  $1.3 \mu\text{A}$ . The PENG device developed from this composite demonstrated a 105-second capacitor charge time, high sensitivity as a pressure sensor (5 kPa), and generated up to 3 V. Overall, output voltage of PENG is nearly five times higher than the pure PVDF film that of the PVDF film alone.



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## Image processing affords temperature mapping using a spin crossover based thermochromic sensor

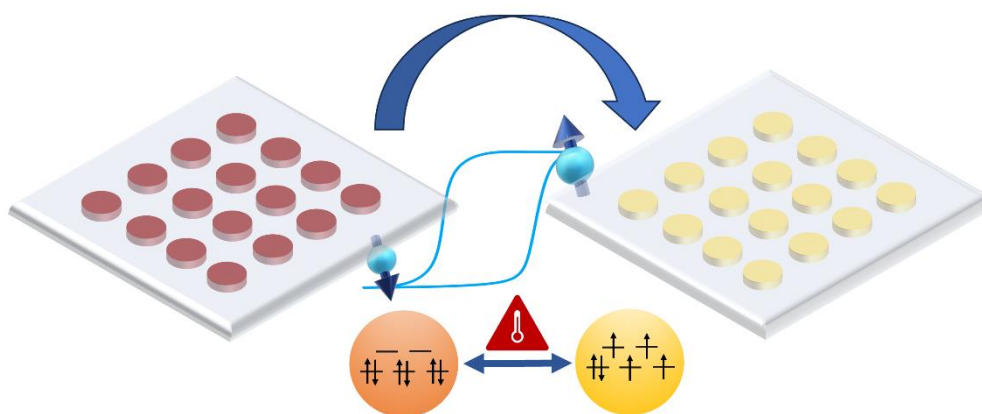
Bhart Kumar<sup>a</sup>, Kamalesh Tripathy<sup>b</sup>, Mitradip Bhattacharjee<sup>b</sup> and Sanjit Konar<sup>a\*</sup>

<sup>a</sup> Department of Chemistry, IISER Bhopal

<sup>b</sup> Electrical Engineering and Computer Science, IISER Bhopal

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The thermochromic behaviour of spin crossover complexes is a desirable feature for non-invasive thermometry technologies.<sup>1-2</sup> Harnessing this, we have developed an easy-to-use flexible sensor label. The proposed prototype is the first of its type, comprising the SCO complex embedded in a transparent PDMS substrate through the mould casting method. The fabrication strategy does not affect the chemical integrity of the complex used, rendering its applicability to a wide range of sensitive spin crossover complexes. The molecule used in this work is a novel Hofmann-type coordination polymer {Fe(Quin)[Pt(CN)<sub>4</sub>], where Quin = quinazoline, that exhibits SCO around ambient conditions with 20 K hysteretic memory. The working principle of the device is based on the thermochromism of the sensing material due to spin transition, which is calibrated through image analysis.<sup>3</sup> The sensor label is tested for a variety of applications, such as (a) smart packaging, (b) temperature mapping, and (c) heat flow monitoring. All these trials have demonstrated the versatile nature of the prototype, establishing its capacity to operate in a wide range of real-life applications.



**Figure.** Schematic representation of thermochromism associated with spin state switching in Fe(II) complexes.

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## Metal- $\pi$ Interaction: An Unconventional Approach Towards Hybrid Material and its Efficacy in Electrocatalytic Reduction of Nitrate to Ammonia

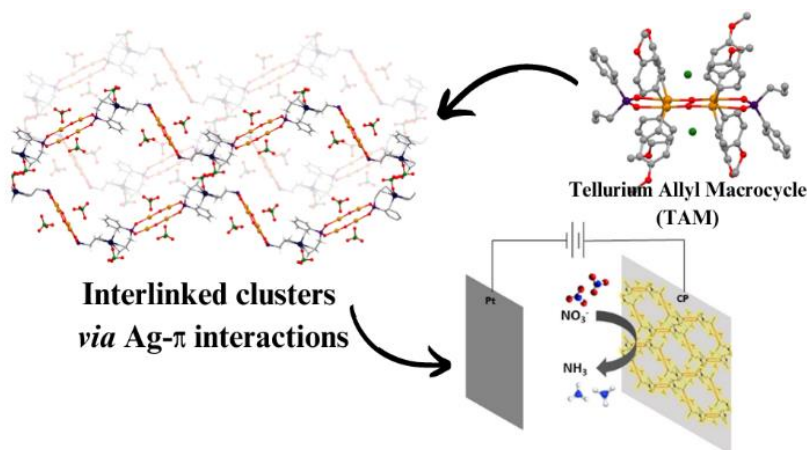
**Calvin Samuel P**,<sup>a</sup> Swandhana V. S,<sup>a</sup> Gujju Narsimhulu,<sup>a</sup> Garima Bangar,<sup>b</sup> Sai Hemanth Kumar Dasari,<sup>a</sup> Gopalan Rajaraman,<sup>b</sup> and Viswanathan Baskar<sup>a\*</sup>

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Enthused by the intriguing nature of metal- $\pi$  interaction in organometallic chemistry, a novel 1D hybrid material has been designed. Here, a functionalized tellurium allyl macrocycle (**TAM**) acts as a molecular building block and is woven together *via* Ag- $\pi$  interaction to obtain **Ag-TAM**. The macrocycle is coordinated to Ag by means of phenyl and allyl groups in  $\eta^2$  mode. **TAM** and **Ag-TAM** were found to be efficient electrocatalysts for the conversion of nitrate to ammonia. **TAM** showed a Faradaic efficiency of 85% and a 60% selectivity towards ammonia. **Ag-TAM** showed an NH<sub>3</sub> yield rate 2-fold greater than **TAM** with a high Faradaic efficiency of 95% and better selectivity of 79%. DFT study unveiled novel mechanistic insights revealing potential cooperative catalysis between neighboring Ag sites, attesting that interlinking of macrocycles *via* Ag- $\pi$  interaction facilitates electron transfer, thus improving the catalytic activity.



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# Synthesis and Isolation of Stable Naphthalenediimide-based Radical Cation and Dication

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Organic radical and radical ions comprise of important class of compounds due to their various application in spin-based synthetic chemistry<sup>1</sup> and material science.<sup>2</sup> However, organic radical ions are highly reactive towards ambient atmosphere, which restrict their applications<sup>3</sup>. In particular, design and synthesis of stable radical cations are attractive since they enable access to strongly electron-deficient organic scaffolds. The first isolated radical cation is Wurster's Blue (**WB<sup>•+</sup>**, 1879). After prolonged efforts, we were able to generate the NDI radical cation, though only in the solution state in (2012).<sup>5</sup>

This study presents the first stable radical cation and dication of a naphthalenediimide- based system both successfully isolated as single crystals through controlled oxidation. We achieved the formation of highly stable NDI radical cation and dication, which maintain the structural integrity in both solid and solution phase. Single crystal X-ray diffraction analysis provide detailed insights into the molecular geometry and electronic structure of these spin and charge bearing species. Electrochemical and spectroscopic investigations confirmed their distinct redox behavior and remarkably stability and with high molar absorption coefficient. These finding represent a significant advance in the chemistry of Rylene-based systems offering potential for applications in the molecular electronic energy storage and redox active materials.

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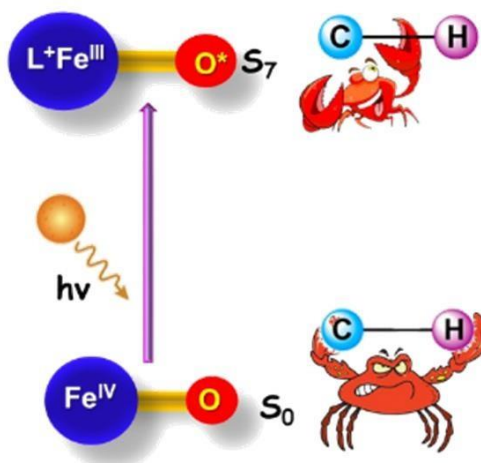
## Effect of spin-state on Photocatalytic Reactivity of Non-Heme Iron(IV)=O Complexes

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High-valent nonheme iron-oxo species, present in both biological enzymes and synthetic systems, are pivotal for C–H bond oxidation and oxygen activation. These complexes, inspired by natural enzymes like bleomycin, provide insights into mechanisms of O<sub>2</sub> and C–H bond activation. Understanding their excited-state chemistry is crucial for designing efficient photo-redox catalysts. In 2017, Browne and colleagues demonstrated that near-UV light excites Fe<sup>IV</sup>=O to [Fe<sup>III</sup>–O\*] complexes, enhancing their reactivity and unlocking new photochemical pathways vital for advanced catalysis<sup>1</sup>. In this study, we investigated the excited-state chemistry of nonheme Fe<sup>IV</sup>=O complexes with benzyl alcohol and ethylbenzene substrates. Browne's work showed that near-UV light increases C–H bond oxidation rates via ligand-to-metal charge transfer (LMCT), forming a reactive [(L<sup>+</sup>)Fe<sup>III</sup>–O\*] species. Our DFT calculations confirmed an intermediate spin state as the ground state of the complex. UV-vis spectra and TDDFT calculations identified an excited state at 694 nm, crucial for the enhanced reactivity and oxyl radical character of Fe<sup>IV</sup>=O complexes. The ground state reactivity exploration reveals that the rate-determining step involves favourable C–H abstraction from the a carbon of the substrate.



**Figure 1** Photocatalytic activation of Fe<sup>IV</sup>=O complex to S<sub>7</sub> excited state (Fe<sup>III</sup>–O\*)

### References:

1 Lawrence Que Jr., Wesley R. Browne et al., *Chem. Commun.*, **2017**, 53, 123571.

# Spin Dynamics and Magnetic Behaviour of Organic Diradicals on Graphene Surface: Insights from computational studies

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In recent years, the magnetic properties of organic diradicals have attracted significant attention from both experimentalists and theoreticians, primarily due to their potential in applications such as spintronics and quantum computing. Despite having weaker magnetic exchange coupling compared to inorganic counterparts, organic systems are particularly appealing because of their longer spin relaxation times, a critical factor for these technologies. To better understand this behaviour, we wanted to focus on the spin dynamics and magnetic properties of these systems. However, for many practical applications, diradicals must be deposited onto surfaces, making it essential to study how their magnetic properties and behaviour are affected in such environments. In this work, we explore the magnetic behavior of experimentally synthesized organic diradicals, when placed onto a graphene surface. We employed density functional theory (DFT) method, to calculate the magnetic properties of the diradical on the surface. The geometry of the diradicals on the graphene surface was fully optimized using the hybrid density functionals. The calculation of the magnetic exchange coupling constant ( $J$ ) was done by the broken symmetry approach given by Yamaguchi. We then calculated the magnetocrystalline anisotropy energy ( $E_{MCA}$ ) and Gilbert damping ( $\alpha$ ), both of which originate from spin-orbit coupling, to analyse the magnetization behaviour and investigate the non-linear spin relaxation phenomenon observed in these magnetic systems. These calculations help in understanding how the rate at which the magnetization reaches equilibrium is controlled, in the case when a diradical is deposited onto a graphene surface. Additionally, we observed that the magnetic properties of the diradical remain intact upon deposition on the surface, as evidenced by the preserved spin density of the diradical.

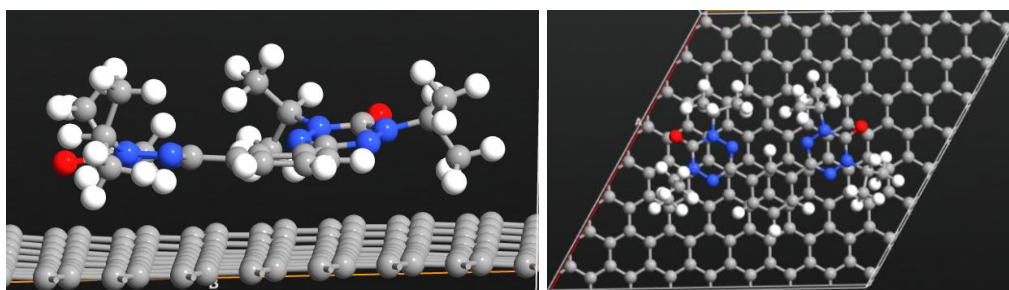
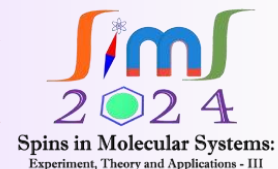


Figure 1: The Diradical on graphene surface (a) side view (b) top view





### Abstract of Poster Presentation of Daniele Sartini:

Stabilizing large easy axis type magnetic anisotropy in molecular complexes is an extremely challenging task, yet it is crucial for the development of molecular-based information storage devices and applications in quantum computing and spintronics. Determining with accuracy the orientation and magnitude of the magnetic anisotropy is extremely difficult, if not impossible, using conventional analytical techniques. Nevertheless, it is essential for understanding the electronic structure and structure-property correlations, which will ultimately facilitate the development of magneto-structural correlations, currently lacking in the literature. In my poster I intend to report a study that I've carried out in collaboration with the group of Professor Maheswaran under the supervision of Prof. Mauro Perfetti. The work is about a series of five-coordinate distorted square pyramidal Co(II) complexes  $[\text{Co}(\text{L})(\text{X}_2)] \cdot \text{CHCl}_3$  (where X = Cl (**1**), Br (**2**), or I (**3**)), all exhibiting axial anisotropy as confirmed by X-band electron paramagnetic resonance (EPR). The value of the axial Zero Field Splitting parameter (D) was quantitatively determined (**1** =  $-72 \text{ cm}^{-1}$ ; **2** =  $-67 \text{ cm}^{-1}$  and **3** =  $-25 \text{ cm}^{-1}$ ) using high-precision cantilever torque magnetometer (CTM). The magnetization relaxation dynamics measurements reveal the presence of field-induced slow relaxation of magnetization due to the predominant Raman relaxation process. Theoretical calculations, in good agreement with the experiments, further elucidate the rationale behind the observed variations in D magnitude and provide insight into the electronic structures of these complexes, suggesting chemical design pathways.



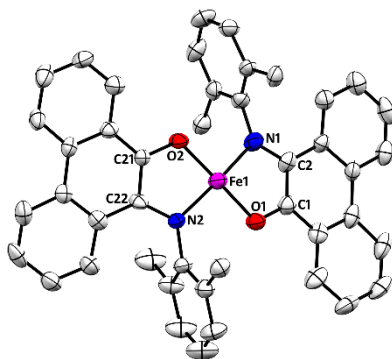
## An Unprecedented Square Planar Fe(III) Complex Exhibiting Spin Crossover Between the Spin-Admixed States

Dipanti Borah, Kamal Uddin Ansari, Maheswaran Shanmugam\*

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The presence of strong spin-orbit coupling, which is comparable to the crystal field in certain ferric-porphyrin/phthalocyanine derivatives, results in a spin-admixed state between the high spin (HS;  $S = 5/2$ ) and intermediate spin (IS;  $S = 3/2$ ) states. However, there are no literature precedents for spin admixing between the intermediate spin (IS;  $S = 3/2$ ) and low spin (LS;  $S = 1/2$ ) states, which are purely governed by axial ligation. It is also true that systems showing spin-admixed behavior do not exhibit thermal equilibrium between the spin states, i.e., spin crossover. Here, we report a unique and rare square planar ferric ion complex,  $[\text{Na}(\text{DME})_3][\text{Fe}(\text{L}^{12-})_2]$  (**1**), which exhibits two different physical phenomena: spin crossover is observed between the spin-admixed states, which is unprecedented. Field- and temperature-dependent Mössbauer spectra, variable temperature X-band EPR spectra, high field EPR (HF-EPR) and temperature-dependent magnetic susceptibility measurements reveal that the spin-admixed state has nearly equal contributions from IS ( $S = 3/2$ ) and LS ( $S = 1/2$ ), unlike other reports in the literature. The detailed electronic structure of **1**, along with the rationale for quantum spin admixing and spin crossover, is well supported by theoretical calculations.



**Figure 1** Thermal ellipsoid picture of the crystal structure of the anionic core of **1**. The hydrogen atoms and side-chain carbon atoms are removed for clarity. Colour code: Magenta = Fe; Red = O, Blue = N and Grey = C.

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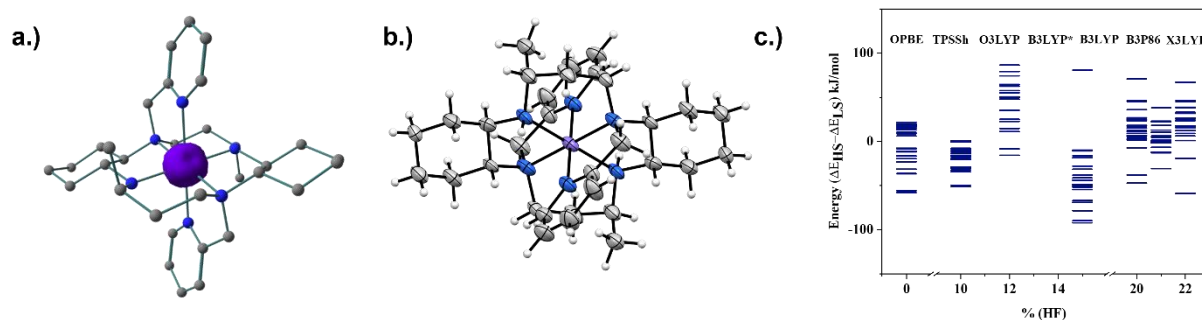
# An In-Depth Evaluation of Systematic Benchmarking of Reported Systems and Synergistic Experimental and Computational Investigation of Fe-tetraazatricyclo Complexes

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The spin-crossover (SCO) molecule belongs to a family of transition metal complexes where the metal can access two different spin configurations because it contains electronic states with different spins but similar electronic energies.<sup>1</sup> Spin cross-over phenomenon is commonly observed with first-row transition metal complexes with a  $d^4 - d^7$  electron configuration. Ligands with  $N_6$  or  $N_4O_2$  donor atoms can act as moderate ligands that are preferable for better SCO behavior.<sup>2</sup> Thus, we are interested in Fe-tetraazatricyclo complexes exhibiting SCO behavior and providing valuable insights into the underlying mechanisms and properties of these fascinating materials. Here we discuss the synthesis of Fe complexes with tetraazatricyclo ligands and the study of their magnetic properties using a SQUID magnetometer and different computational methods, particularly DFT calculations.<sup>3</sup> To further explore the DFT insight in exploring the suitable Hybrid Functional to predict the accurate ground state for the SCO complexes, benchmark studies are performed. Thus, we have selected twenty-six complexes reported with SCO for the same. The seven different hybrid functional (TPSSh, O3LYP, B3LYP\*, B3P86, B3LYP, X3LYP, OPBE) have been chosen according to the percentage amount of their Hartree-Fock exchange. We have compared the experimental and calculated thermodynamic parameters (Enthalpy, Entropy), Transition temperature ( $T_{1/2}$ ), Spin pairing energy, and the difference between the two spin states: High and Low.



**Figure 1;** (a) Spin density diagram for  $[Fe^{II}(TAZC-py)]$  complex. (b) Crystal structure of a  $[Co^{II}(TAZC-py)]$  complex. (c) Energy difference (high-spin – low-spin) for the 26 studied systems plotted against the amount of exact Hartree–Fock mixed into the corresponding exchange-correlation functional.

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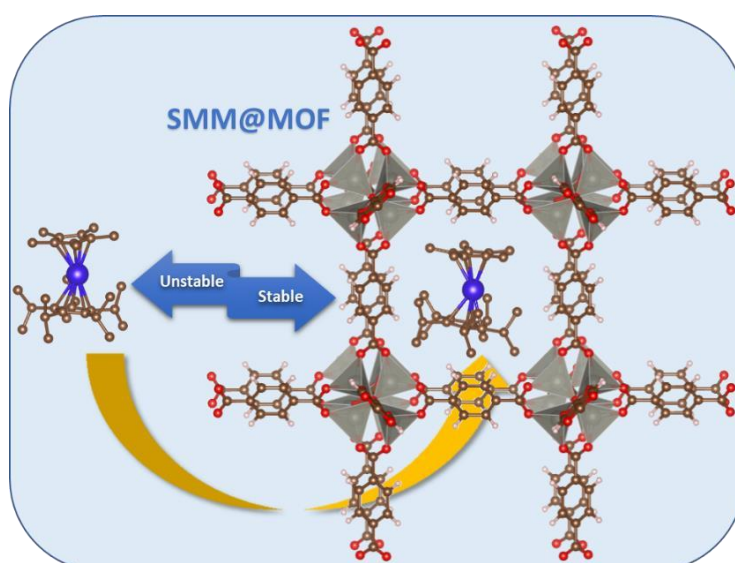
# Achieving Ambient Stability and Suppressing Spin-Phonon Coupling in Dyprosocenium SIMs via MOF Encapsulation

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Detailed ab initio Complete Active Space Self-Consistent Field (CASSCF) calculations, combined with periodic Density Functional Theory (DFT) studies, have been conducted on the  $[(Cp^*)Dy(Cp^{iPr5})]^+$  [1] molecule encapsulated within a metal-organic framework (MOF). These comprehensive analyses revealed that MOF encapsulation significantly enhances the stability of these otherwise fragile molecules while preserving their effective magnetic moment ( $U_{eff}$ ) values. Notably, this encapsulation effectively suppresses the critical vibrational modes typically responsible for reducing the blocking temperature. [2] This suppression presents a previously unexplored strategy for developing a new generation of Single-Molecule Magnet (SMM)–based devices, potentially revolutionising the field.



**Figure 1** Achieving stability of Dy-based SMM complex upon MOF encapsulation.

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## Synthesis and Electronic Structure Studies of an Ytterbium-Pyrazine Square complex

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Molecule based materials offer a promising platform for the discovery of emergent physical properties by fine tuning of metal-ligand frontier orbital overlap and associated redox potentials.<sup>1,2</sup> Nitrogen bases such as bipyridine, triazine, pyrazine etc can lead to various multi-metallic or polymeric molecule based materials.<sup>1,3</sup> Among these, pyrazine- based compounds and materials have gained interest in recent years in studying strong electron correlations, single molecule magnetism and other unique electronic properties.<sup>4-6</sup> These physical properties in such compounds arise due to reduced pyrazine concurrent with judiciously chosen metal ions. For example, samarium salt ( $\text{SmI}_2$ ) reduces pyrazine to form a 1D chain and shows valence tautomeric behavior. However,  $\text{YbI}_2$  does not reduce pyrazine despite of forming isostructural chain.<sup>7</sup>

We hypothesized that organo-ytterbium complexes with known and controllable redox potential can be used as a precursor to reduce pyrazine by metal-ligand redox cooperativity. We and others have previously shown that metal-ligand redox cooperativity can significantly alter the redox potential of donor and acceptors upon coordination.<sup>8</sup> Successfully building up on this idea, we have used a divalent monomeric ytterbium source  $[(\text{C}_5\text{H}_4\text{Me})_2\text{Yb}(\text{THF})_2]$  (1) to reduce pyrazine forming a multi-metallic square complex  $[(\text{C}_5\text{H}_4\text{Me})_2\text{Yb}(\text{pyrazine})]_4$  (2) by coordination induced potential shift. The characterization and electronic structure of this square complex is studied by Single-crystal X-ray diffraction, X-ray absorption spectroscopy, magnetometry, and calculations among other techniques.

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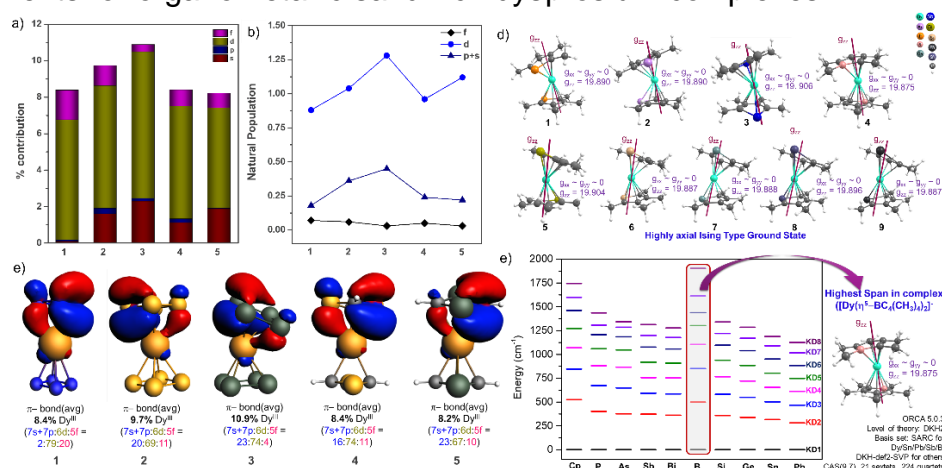
# Unravelling Electronic Structure, Bonding, and Magnetic Properties of Dysprosium Complexes

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Single Molecule Magnet (SMM) is a class of molecules that can potentially retain its magnetization at low temperatures. The application of SMM ranges from storage devices to quantum computing. Dy(III) ion plays an increasingly important position in SMM research with its total orbital angular momentum  $J = 15/2$ , which can create large magnetic anisotropy. In the last decade, researchers have been exploring high-performance Dy(III)-based SMMs via effectively suppressing the Raman and QTM, which are detrimental to magnetic relaxation, by designing ligands with expected crystal fields and maintaining local high symmetry of metal centers<sup>1,2</sup>. In this work, we have studied sandwich complexes of Dy(III) viz.  $[\text{Dy}(\text{E}_4)_2]^-$  (where E = N, P, As, CH) and  $[\text{Dy}(\text{EC}_4(\text{CH}_3)_4)_2]^{+/-}$  (where E = BCH3, C, Si, Ge, Sn, Pb, P, As, Sb, and Bi) using DFT and *ab initio* methods to compute the spin Hamiltonian (SH) parameters (D tensor and g tensor). The four-member ring is the smallest stable ring, so it better stabilizes the axial anisotropy thus making  $[\text{Dy}(\text{N}_4)]^-$  the most anisotropic complex.<sup>3</sup> We were able to predict the performance of these molecules as SMMs, with estimated energy barrier (Ucal) values >2000 K, making them potential highly efficient carbon-free replacements for organometallic sandwich dysprosium complexes.



**Figure 1:** (a) DFT computed %M contribution to Dy-E NLMOs for complexes  $[\text{Dy}(\text{E}_4)_2]^-$ , (b) NBO computed Natural Population Analysis for complexes  $[\text{Dy}(\text{E}_4)_2]^-$ , (c) The Dy-E bonding NLMOs along with %M contribution to NLMOs for complexes  $[\text{Dy}(\text{E}_4)_2]^-$ , (d) CASSCF computed the orientation of the main magnetic  $g_{zz}$  axes for complexes  $[\text{Dy}(\text{EC}_4(\text{CH}_3)_4)_2]^{+/-}$  and (e) SINGLE\_ANISO computed splitting in the low-lying eight KDs for complexes  $[\text{Dy}(\text{EC}_4(\text{CH}_3)_4)_2]^{+/-}$

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## Rational Design of Ferromagnetic Graphene by Selective Hydrogenation

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Though functionalized graphene have revolutionized technology in several domains, their magnetic utility remains explorative. Computationally, alternating sp<sup>3</sup> and sp<sup>2</sup> carbon is predicted to exceed the magnetization of  $\alpha$ -Fe<sup>1</sup>, and show ferromagnetic ordering in graphene<sup>2</sup>. However, the electronic and topological origins of the observed magnetic ordering in hydrogenated graphene remain mysterious<sup>3</sup>. Here, we show that introducing a sp<sup>3</sup> defect in the graphene by hydrogenation radicalizes its three para carbons due to the formation of Clar's sextets<sup>4</sup> on the hexagonal rings incident to the defect. Further sp<sup>3</sup> defects that reinforce radical sites lead to a ferromagnetic spin-flip band-gap and higher curie (T<sub>c</sub>) temperature. The Origin of stability arises from the planar triphenyl methyl radical microstructure where the phenyl ring has radicals substituted at its meta positions.

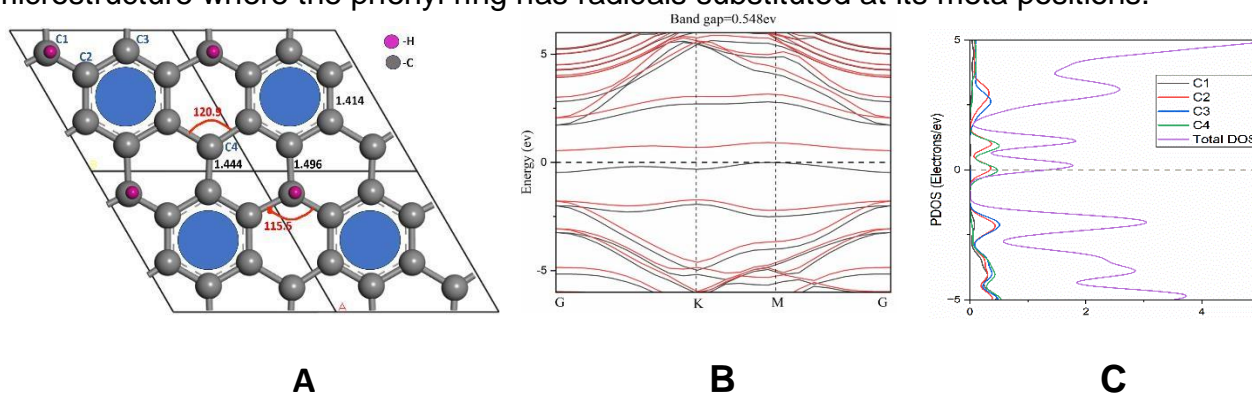


Figure 1 Structure of the DFT optimized (a) Ferromagnetic unit cell of C<sub>6</sub>(C)(CH) 2D hexagonal network, its (b) Ferromagnetic band structures (c) and atom projected DOS.

Besides providing the origin of stability for the ferromagnetic ordering experimentally observed in the hydrogenated graphene, our results provide a clear structural motif for the bottom-up synthesis of magnetized graphene derivatives with chemical rationale.

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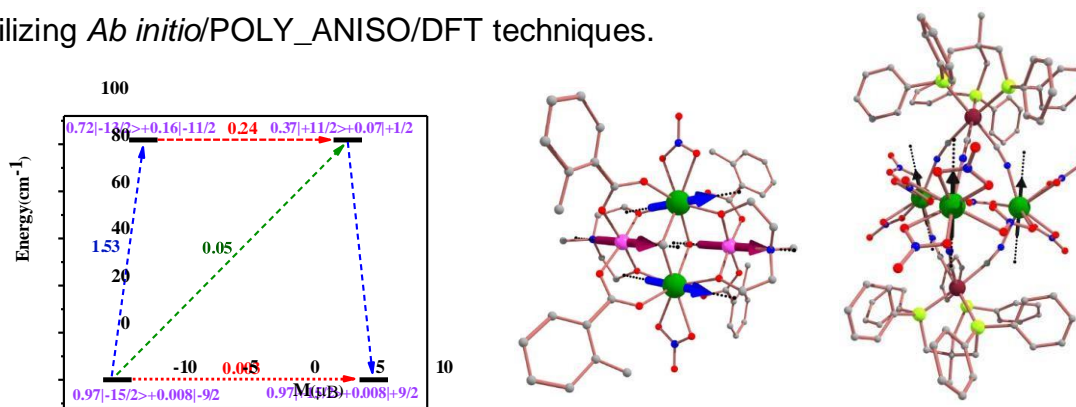
## In pursuit of 4d/5d-4f Single Molecule Magnets

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To enhance the SMM properties, larger magnetic exchange interactions are very necessary since they can help reduce the quantum tunneling of magnetization (QTM), which has become essential for polynuclear systems. 4d and 5d ions are preferred instead of their comparable 3d–4f and 4f–4f counterparts because these ions are more anisotropic and have more diffused d orbitals, which may encourage stronger magnetic exchange<sup>1-2</sup>. We herein present the synthesis, crystal structure, and computational analysis of a Ru<sub>2</sub>Ln<sub>2</sub> butterfly metallic core complex having molecular formula [Ru<sup>II</sup><sub>2</sub>Ln<sup>III</sup><sub>2</sub>(OMe)<sub>2</sub>(*ortho*-tol)<sub>4</sub>(mdea)<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>] (*ortho*-tol = *ortho*-toluate, mdeaH<sub>2</sub> = N-methyldiethanolamine) [Ln= Dy(**1**), Ho(**2**), Tb(**3**), Gd (**4**), and Er (**5**)]. *Ab initio* calculations resulted in a calculated energy barrier ( $U_{cal}$ ) of 101.8 cm<sup>-1</sup> for Dy<sup>III</sup> metal ions in **1** and negligible  $U_{cal}$  for **2** and **5**. DFT calculations yielded exchange coupling values of  $-1.32$  cm<sup>-1</sup> of  $J_1$ (Gd-Ru),  $0.01$  cm<sup>-1</sup> for  $J_2$  (Gd-Gd) and  $-0.24$  cm<sup>-1</sup> of  $J_3$  (Ru-Ru). Furthermore, we will present the computational analysis to calculate the energy barrier and exchange interaction between the metal centers for trigonal bipyramidal (TBP) compounds (Et<sub>4</sub>N)<sub>2</sub>[(triphosRe(CN)<sub>3</sub>)<sub>2</sub>(Ln(NO<sub>3</sub>)<sub>3</sub>)<sub>3</sub>]·4CH<sub>3</sub>CN {Ln = Tb (**6**) and Dy (**7**)<sup>3</sup> by utilizing *Ab initio*/POLY\_ANISO/DFT techniques.



**Figure 1.** The *ab initio* computed magnetization blocking barrier for Dy1 centre of complex **1** (left). Magnetic anisotropy directions of complex **1** (middle) and **7** (right).

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## Decoding the Electronic Origins of Outer-Sphere & Inner-Sphere Electron Transfer in High-Valent Non-Heme Metal-oxo Species

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The electron transfer (ET) step is one of the crucial processes in biochemical redox reactions that occur in nature. Although metalloenzymes possessing metal-oxo units at their active site are typically associated with outer-sphere electron transfer (OSET) processes, biomimetic models, in contrast, have been found to manifest either an inner-sphere electron transfer (ISET) or OSET mechanism. This distinction is clearly illustrated through the behaviour of  $[(N4Py)Mn^{IV}(O)]^{2+}$  (**1**) and  $[(N4Py)Fe^{IV}(O)]^{2+}$  (**2**) complexes, where complex **1** showcases an OSET mechanism, while complex **2** exhibits an ISET mechanism, in their reactions involving C-H bond activation and oxygen atom transfer reactions in the presence of a Lewis acid.<sup>1</sup> However, the precise reason for this puzzling difference remains elusive. Our calculations indicate that when the substrate (toluene) approaches both **1** and **2** that is hydrogen bonded with two HOTf molecules (denoted as **1-HOTf** and **2-HOTf**, respectively), proton transfer from one of the HOTf molecules to the metal-oxo unit is triggered and a simultaneous electron transfer occurs from toluene to the metal centre.<sup>2</sup> Interestingly, the preference for OSET by **1-HOTf** is found to originate from the choice of  $Mn^{IV}=O$  centre to abstract spin-down ( $\beta$ ) electron from toluene to its  $\delta(d_{xy})$  orbital. On the other hand, in **2-HOTf**, a spin state inversion from triplet to quintet state takes place during the proton (from HOTf) coupled electron transfer (from toluene) preferring a spin-up ( $\alpha$ ) electron abstraction to its  $\sigma^*(d_{z^2})$  orbital mediated by HOTf giving rise to ISET. In addition, **2-HOTf** was calculated to possess a larger reorganisation energy, which facilitates the ISET process via the acid. The absence of spin-inversion and smaller reorganisation energy switch the mechanism to OSET for **1-HOTf**. Therefore, for the first time, the significance of spin-state and spin-inversion in the electron transfer process has been identified and demonstrated within the realm of high-valent metal-oxo chemistry.

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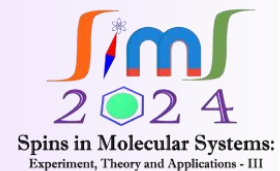
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**MODERN TRENDS IN MOLECULAR MAGNETISM – IV  
&  
SPINS IN MOLECULAR SYSTEMS:  
EXPERIMENT, THEORY AND APPLICATIONS – III**



**K. Vignesh (IIT Bombay)**



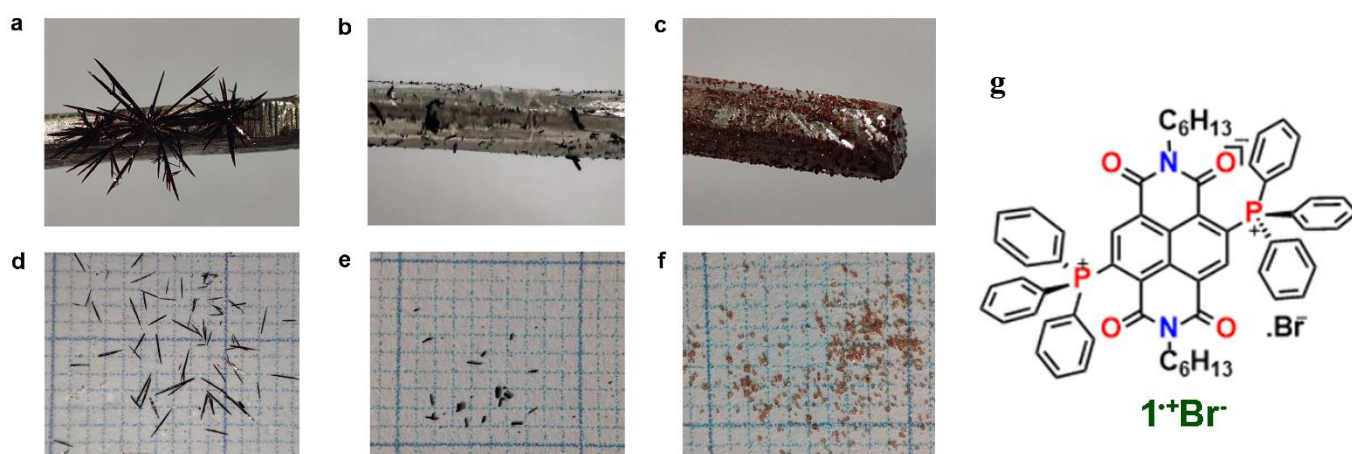
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## Multiple redox-states crystallized by controlled electrocrystallization

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In this research, we are presenting a pioneering study on the Electrocrystallization of all the three Direduced, Radical cation and Dication redox states of a novel class of Naphthalene Diimide (NDI) molecules. The electrocrystallization process, driven by controlled electrical energy, allowed for the controlled growth of well-organized crystalline structures of these unique molecular redox states. To the best of our knowledge, this marks the first instance of obtaining multistate crystals of this profusely tunable arylene group of molecules through electrocrystallization. The experimental UV-Vis NIR absorption spectroscopic, single crystal X-ray diffraction data demonstrates the successful synthesis of these crystal forms and provides insights into their morphological and structural characteristics. Conductivity studies show all states are highly insulating and The results highlight the potential of electrocrystallization and it could pave the way to a milestone for getting all the three redox states of molecular crystal through electrocrystallization.



**Figure 1:** a), b) & c) are the crystals grown on electrode and d), e) & f) are the harvested crystals on graph sheet of  $1^{2\pm}$ ,  $1^{+\cdot}\text{PF}_6^-$ , &  $1^{2+}2\text{PF}_6^-$  respectively. g) is the structure of  $1^{+\cdot}\text{Br}^-$ .

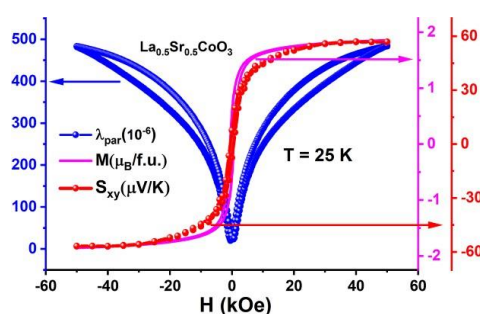
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## Anomalous Nernst Effect and Giant Magnetostriction in Microwave processed $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_3$

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Anomalous Nernst effect (ANE) occurs when a ferromagnet generates a thermoelectric voltage perpendicular to the temperature gradient and applied magnetic field<sup>1</sup>. This permits magnetic metals and alloys to generate electricity from heat. Reports on ANE in oxides are scarce than metallic alloys. This study examines ANE and magnetostriction in microwave-synthesized perovskite oxide  $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_3$ .  $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_3$  is ferromagnetic below its Curie temperature ( $T_C$ )  $\sim 247$  K and metallic resistance. Its main charge carriers are electrons. The Nernst coefficient ( $S_{xy}$ ) has a magnetic field dependency similar to magnetization at a constant temperature below  $T_C$ . The anomalous contribution to  $S_{xy}$  peaks at  $0.21 \mu\text{V/K}$  at  $180$  K and  $H = 50$  kOe. The data analysis suggests that skew scattering occurring in a bad metallic regime may cause the ANE in this sample. The magnetostriction is positive, which means that the sample elongates in the direction of the applied magnetic field. The fractional change in length is  $500$  ppm at  $H = 50$  kOe and at  $T \leq 40$  K. This value is high compared to other  $3d$  perovskite oxides<sup>3</sup>. The giant magnetostriction in this compound is not only caused by spin-orbit scattering induced by the field but also by structural modifications. ANE and giant magnetostriction in a single material is intriguing for thermal energy harvesting and actuator applications.



**Figure 1** Magnetic field-dependent magnetization, magnetostriction and ANE.

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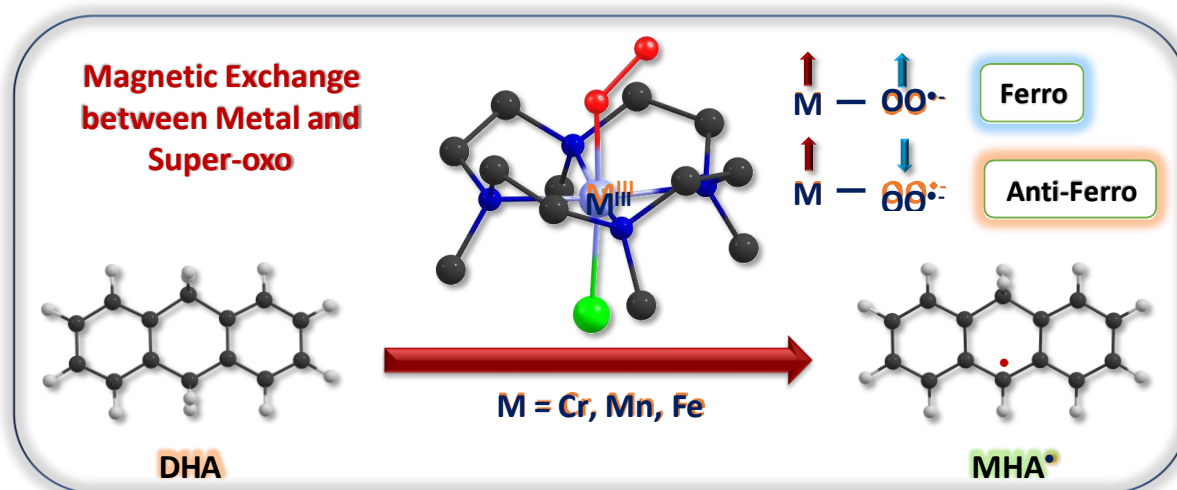
# Unveiling the Role of Magnetic Exchange in Metal–Superoxo Species for C–H Bond Activation Reactions

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Metal–superoxo species are widespread in metalloenzymes and bioinorganic chemistry, recognized for their high reactivity and capacity to activate inert C–H bonds.<sup>1–3</sup> However, chemical properties of the metal-superoxo species have been less clearly understood and still remain elusive in many aspects.<sup>4</sup> This work probes into our efforts using state-of-the-art DFT approach to unveil geometrical, spin state energetics, electronic structures and mechanistic intricacies underlying the activation of C–H bonds by high-valent metal-superoxo catalytic systems. Furthermore, we have shed light on the role of magnetic exchange on the barriers associated with C–H bond activation. A comparison of the oxidative abilities of M–O<sup>•−</sup> species (M = Cr<sup>3+</sup>, Mn<sup>3+</sup>, and Fe<sup>3+</sup>) in C–H bond activation reactions is presented. DFT calculations show that Fe<sup>3+</sup>– and Mn<sup>3+</sup>–superoxo species are more potent oxidants than Cr<sup>3+</sup>–superoxo species, suggesting that their reactivity may be linked to the magnetic exchange parameter. This work presents a glimpse of endeavors within the field of inert C–H bond activation reactions through the utilization of high-valent metal-superoxo species.



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## Magnetic Coupling and Spintronics properties of Helical Phenalene Diradicals

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Phenalene (triangulene), a zigzag-edged odd alternant hydrocarbon unit has attracted significant attention due to its unique electronic properties. When adopting a helical structure, phenalene exhibits chirality, a feature that is increasingly relevant for applications involving the chiral-induced spin selectivity (CISS) effect. While isolated phenalene exists in a doublet ground state, its dimers can exist either singlet or triplet ground states depending on the coupling position. In this study, we have designed helical phenalene-based diradicals coupled through conjugated molecular linkers. Density functional theory (DFT) calculations using the broken symmetry approach, as proposed by Noodleman and Yamaguchi, reveal both ferromagnetic and antiferromagnetic coupling in these diradicals. The diradicals follow the spin alternation rule of magnetic coupling. To explore the spintronic properties, we analysed the transmission spectra and current-voltage (I-V) characteristics of the diradicals. Notably, some of these systems exhibit promising spin-filtering behaviour, making them potential candidates for spintronic applications. This study provides new insights into the design of chiral molecular magnets and their role in spintronics, expanding the utility of helical phenalene diradicals in designing molecular chiral magnets.

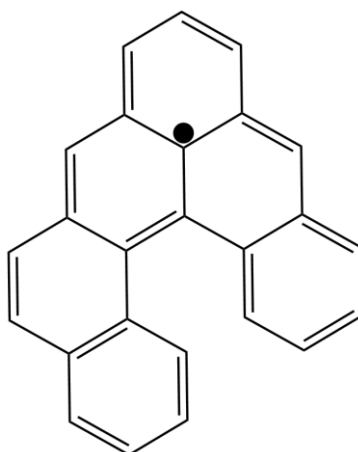


Figure 1. Helical phenalenyl radical

## Efficient Water Splitting with a Semi-conductor based Supramolecular Catalyst

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Photo-electrochemical water splitting is a promising approach for the sustainable production of hydrogen fuel using the solar energy. However, a major challenge lies in identifying an efficient catalyst for overall water splitting reaction, as the multi-electron transfer processes associated with water oxidation are kinetically slow over most of the semi-conductor catalysts. Consequently, integrating photoactive semi-conductors with an active co-catalyst for water oxidation is widely regarded as an effective strategy to enhance catalytic efficiency. In this study, we focus employing a host-guest supramolecular co-catalyst anchored on Bismuth Vanadate ( $\text{BiVO}_4$ ), an efficient photo-anode material due to its favorable band gap as an oxygen evolution reaction (OER) catalyst. Cucurbiturils (CB), macrocyclic compounds have the ability to coordinate with metal ions through its carbonyl portals, is selected as a host molecule. We consider CB[5], which is physisorbed onto the  $\text{BiVO}_4$  surface and subsequently functionalized with earth-abundant metal ions ( $\text{Co}^{2+}$ ,  $\text{Fe}^{2+}$ , and  $\text{Ni}^{2+}$ ) immobilized at its carbonyl portals, resulting in a robust catalytic system for enhanced photo-electrochemical water splitting. Among the three metal ions considered,  $\text{Co}^{2+}$  containing system is found to have the better catalytic activity with lowest overpotential for OER. Our computed energy profiles for water oxidation provide valuable insights to experiments.

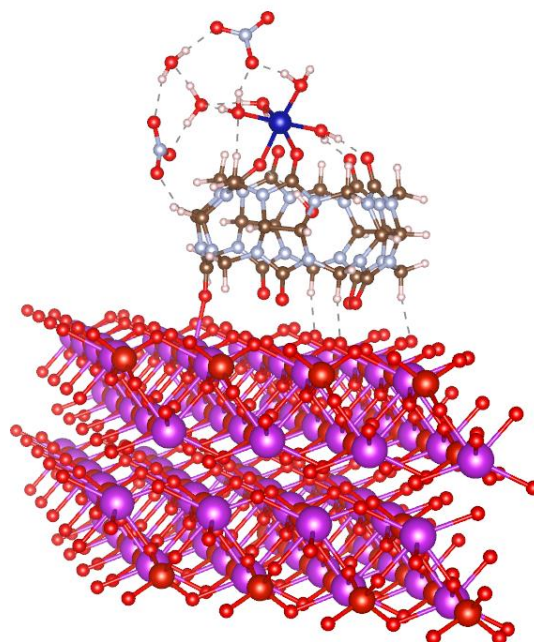


Figure 1  $\text{M}^{2+}$ -CB[5]  $\text{BiVO}_4$  Catalyst

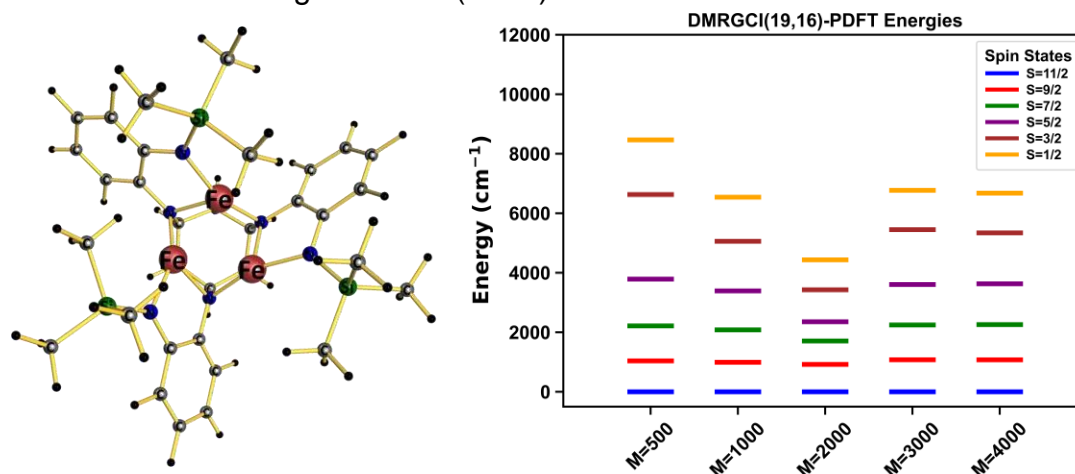
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# Deciphering the Origin of Double Exchange and Magnetic Exchange in a [Fe<sub>3</sub>] Cluster using Density Matrix Renormalization Group (DMRG) Approach

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Multinuclear transition metal clusters have significant potential for small molecule activation, electron transfer in biological systems, and magnetic data storage devices. In particular, mixed-valence iron clusters are known to couple spin components through double-exchange, stabilizing high-spin states. This unique property makes them highly suitable for applications as single-molecule magnets.<sup>1,2</sup> In this study, a combination of advanced multireference methods, including Density Matrix Renormalization Group configuration interaction (DMRG-CI), multiconfiguration pair density functional theory (MC-PDFT), and state-averaged complete active space self-consistent field (SA-CASSCF), was employed to investigate a mixed-valence trimeric iron cluster, [(18-C-6)K(thf)<sub>2</sub>][(<sup>tb</sup>S)LFe<sub>3</sub>]<sup>3</sup>. These methods helped identify key properties as spin ladder, double exchange, and zero-field splitting of the complex. A very strong double exchange interaction with  $B = 230 \text{ cm}^{-1}$  was obtained from SA-CASSCF(19,16) calculation which is in excellent agreement with the experimental maximum of  $\sim 250 \text{ cm}^{-1}$  from the intra-valence charge transfer (IVCT) band.



**Figure 1** Crystal structure of the [(<sup>tb</sup>S)LFe<sub>3</sub>]<sup>-</sup> (left) and the DMRGCI-PDFT computed spin ladder of the molecule (right).

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**MODERN TRENDS IN MOLECULAR MAGNETISM – IV  
&  
SPINS IN MOLECULAR SYSTEMS:  
EXPERIMENT, THEORY AND APPLICATIONS – III**



**Neha Sharma**



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## Self-Assembly of Cyano-Bridged [CoFe] Molecular Dimers: Synthesis and Characterization

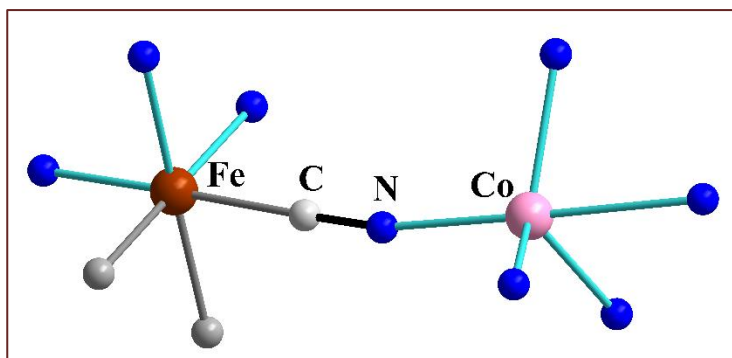
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The constant pursuit for more compact high-tech gadgets has led to a great deal of research interest in advanced multifunctional molecule-based materials.<sup>1</sup> Prussian blue and its derivatives, have emerged as promising candidates for the fabrication of multifunctional molecular materials. Molecular Prussian blue analogues (PBAs) having M-CN-M', cyanide linkages between two transition metals, display a variety of fascinating magnetic properties along with electron transfer coupled spin transition (ETCST) in response to external stimulants like light, temperature, pressure, magnetic or electric fields, etc.<sup>2</sup>

We have recently designed two cyano-bridged Co-Fe discrete molecular dimers,  $[\{\text{Co}(\text{Me}_2\text{TPA})(\mu\text{-NC})\text{Fe}(\text{Tp}^*)(\text{CN})_2\}][\text{Fe}(\text{Tp}^*)(\text{CN})_3]$  (**1**) and  $[\{\text{Co}(\text{NTB})(\mu\text{-NC})\text{Fe}(\text{Tp}^*)(\text{CN})_2\}](\text{ClO}_4)$  (**2**) ( $\text{Tp}^*$  = hyrotris(3,5-dimethylpyrazol-1-yl)borate,  $\text{Me}_2\text{TPA}$  = tris(3,5-dimethylpyrazol-1-ylmethyl)amine and NTB = Tris(2-benzimidazolymethyl)amine) utilizing *fac*- tricyanido building block. In both the eventual possible smallest PBAs, the geometry around the Co centre is fascinatingly trigonal bipyramidal (TBP). Complex **1** and **2**, has been characterized by elemental analysis, spectroscopy, structural, UV-Visible and electrochemical analysis.



### References:

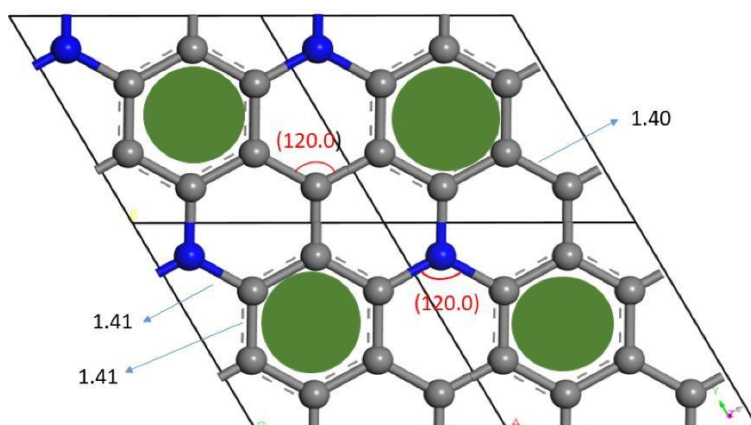
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## In silico Investigation of Magnetic Properties of Heteroatom-doped Graphene (C<sub>7</sub>X, X= N, B)

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Graphene-based systems have gained significant attention for spintronic technologies, where electron spin can be harnessed for computational logic, communication, and information storage<sup>1</sup>. Several theoretical and experimental studies highlight the importance of inducing magnetism in graphene structures<sup>2</sup>. Among them, the substitutional doping of some carbon atoms with electron-rich<sup>3</sup> N and electron-poor<sup>4</sup> B appears to be promising. Here, we conduct an in-depth inquiry into the chemical impact of doping 1/8th of carbons with hetero atoms that leads to a C<sub>7</sub>X unit cell (Figure). This allows the odd electron to acquire stability by delocalizing over the adjacent aromatic rings, which are constrained to be in the plane by the network topology.



**Figure 1:** The hexagonal unit cell of C<sub>7</sub>X illustrated with Nitrogen doping.

Our work unveils the chemical impact of the empty p<sub>z</sub> orbital of boron and the lone pair of nitrogen on the unpaired electron delocalization and the resulting magnetic properties.

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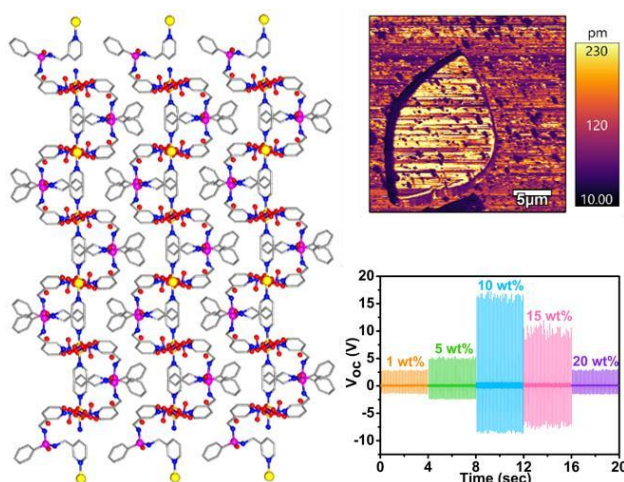
# A Ferroelectric Two-Dimensional Metal-Organic Coordination Polymer Showing Piezoelectric Energy Harvesting Properties

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Ferroelectric materials with switchable polarization are promising for piezoelectric nanogenerators (PENGs). In this context, metal-ligand systems due to their tunable structure, low toxicity, flexibility, and ability to incorporate polarizable dipolar groups, making them suitable for advanced energy and electronic applications. This study explores the development of piezoelectric nanogenerators (PENGs) using a two-dimensional metal-ligand coordination polymer, [Cu(PhPONHCH<sub>2</sub>(<sup>3</sup>Py)<sub>2</sub>](NO<sub>3</sub>)<sub>2</sub>·2H<sub>2</sub>O (**1**), synthesized with a noncentrosymmetric dipodal ligand. This polymer exhibits ferroelectricity through the displacement of a weakly bonded counteranion nitrate, facilitated by the framework's flexibility. Piezoresponse force microscopy (PFM) reveals an impressive longitudinal piezoelectric coefficient (*d*<sub>33</sub>) of 82 pm/V, unprecedented for metal-organic frameworks (MOFs). Composites of **1** with thermoplastic polyurethane (TPU) demonstrate excellent PENG performance, achieving a maximum output voltage of 25.05 V and a power density of 48.69 μW/cm<sup>2</sup> for the optimized 10 wt% (**1**-TPU) device. These findings highlight the potential of MOFs in renewable energy applications and contribute to the understanding of polarization mechanisms in coordination polymers.



**Figure 1** A polar 2-D coordination polymer exhibiting high direct and inverse piezoelectricity in the form of PENGs

## References:

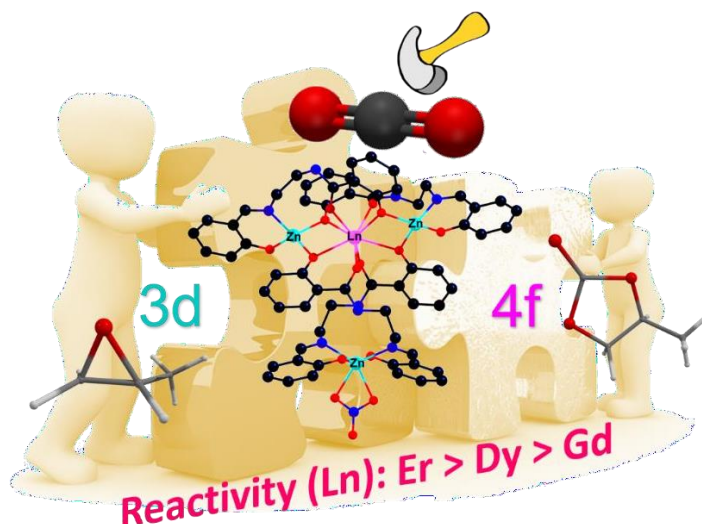
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# Unravelling the Mechanism of CO<sub>2</sub> Activation: Insights into Metal-Metal Cooperativity and Spin-Orbit Coupling with {3d–4f} Catalysts

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Converting CO<sub>2</sub> into useful chemicals using metal catalysts is a significant challenge in chemistry. Among the various catalysts reported, transition metal lanthanide hybrid {3d–4f} complexes stand out for their superior efficiency and site selectivity. However, unlike transition metal catalysts, understanding the origin of this efficiency in lanthanides poses a challenge due to their orbital degeneracy, rendering the application of DFT methods ineffective. In this study, we employed a combination of density functional theory (DFT) and ab initio CASSCF/RASSI-SO calculations to explore the mechanism of CO<sub>2</sub> conversion to cyclic carbonate using a 3d–4f heterometallic catalyst for the first time. This work unveils the importance of 3d and 4f metal cooperativity and the role of individual spin-orbit states in dictating the overall efficiency of the catalyst.



**Figure 1** CO<sub>2</sub> activation using 3d-4f catalyst showing metal-metal cooperativity and role of spin-orbit coupling in catalytic efficiency.

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# The Interplay of Spin States, Ligands, and Additives in High Valent Metal–Oxo Mediated C–H Activation: A Computational Study

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High-valent metal–oxo intermediates are key species in metal-oxygen chemistry, playing a central role in various biological processes such as photosystem-II, naphthalene dioxygenase, and peroxidases. For instance, high-valent iron-oxo species are integral to the catalytic cycles of both heme and non-heme iron enzymes, facilitating the insertion of an oxygen atom from dioxygen into the inert C–H bonds of aliphatic and aromatic hydrocarbons. In heme iron enzymes like cytochrome P450, Fe<sup>IV</sup>=O cation radical porphyrin compound I (Cpd I) and Fe<sup>IV</sup>=O porphyrin compound II (Cpd II) are proposed as the reactive intermediates. Of these, Cpd I has been extensively studied for its biological significance, while Cpd II has also been shown to activate C–H bonds in alkanes. Cpd I is more reactive than Cpd II, a difference attributed to variations in their spin states. The Fe<sup>IV</sup>=O species in metalloenzymes typically exhibit a high-spin (S=2) ground state, while biomimetic Fe<sup>IV</sup>=O species generally favor a triplet (S=1) spin state, with some exceptions. To better understand and control the reactivity of these species, numerous model complexes have been synthesized in the laboratory to replicate the behavior of metalloenzymes. Both experimental and theoretical approaches have been employed to investigate the C–H bond activation capabilities of heme and non-heme model complexes.<sup>1-3</sup> Using computational methods, present study aims to address the following questions: (i) Does the individual spin state influence C–H bond activation? (ii) How does geometry and ligand architecture affect the nature of the metal–oxo species? (iii) Do additives decrease the C–H activation barrier?

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## Mechanistic investigations of C-H activation by various spin states of $[\text{Co}^{\text{III,IV}}_2(\mu\text{-O})_2]$ diamond core complex

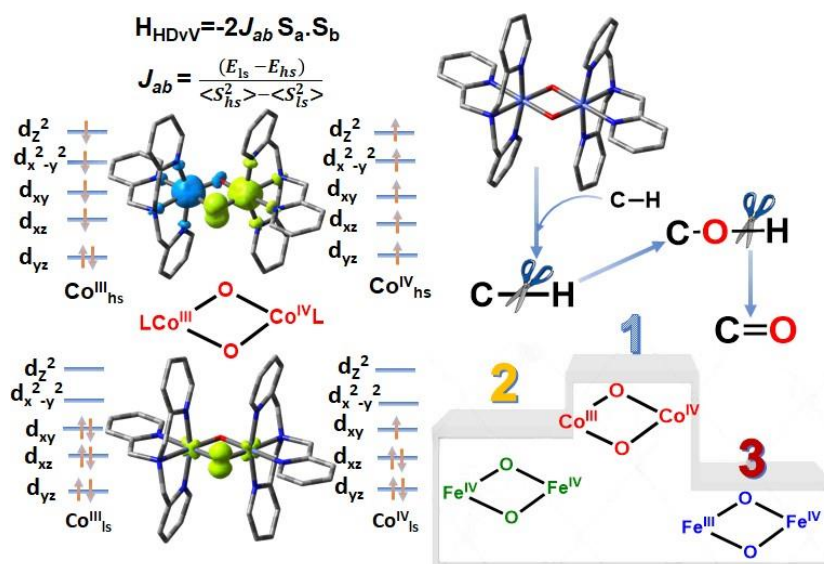
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C-H activation is a key biochemical process often facilitated by heme and nonheme enzymes through high-valent metal-oxo species. Among these, nonheme dinuclear iron-dependent enzyme, soluble methane monooxygenase (sMMO), stands out for its ability to activate strong C-H bonds via a diiron(IV) intermediate<sup>1</sup>. Our study focuses on a cobalt diamond core complex  $[\text{Co}^{\text{III,IV}}_2(\mu\text{-O})_2]$  supported by a tris(2-pyridylmethyl)amine (TPA) ligand, which has been experimentally proven to have a remarkably high rate constant for C-H bond activation in 9,10-dihydroanthracene (DHA), surpassing analogous first-row transition metal complexes, including the well-established diiron systems<sup>2</sup>. Employing Broken Symmetry Density Functional Theory (BS-DFT) and Complete Active Space Self-Consistent Field (CASSCF) methods, we have theoretically investigated the mechanistic pathways through the prism of multi-state reactivity and unearthed the electronic factors driving such C-H activation process. Comparative barrier analyses between cobalt and iron diamond core complexes further reveal the distinctive advantages of the cobalt system in understanding metal-oxo mediated hydrogen abstraction.

**Figure1:** Schematic representation of the work



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# A Machine Learning Approach to Decipher the Origin of Magnetic Anisotropy in Three-Coordinate Cobalt Single-Ion Magnets

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Single Molecule Magnets (SMMs) serve as vital models for permanent magnets and are key to compact information storage and molecular spintronics. A critical factor in SMM behavior is magnetic anisotropy, especially the axial zero-field splitting parameter ( $D$ ) in mononuclear transition metal complexes.[1] Low-coordinate mononuclear complexes, in particular, exhibit higher anisotropy and blocking temperatures compared to other molecular classes. However, predicting the sign and magnitude of the  $D$  value is a challenging task due to the influence of donor atom properties and structural parameters.[2] To address this, an initial dataset of 90 Co(II) complexes was curated and expanded to 614 complexes through optimization techniques. Attempts to predict  $D$  values and their classifications using traditional magneto-structural correlations were inadequate. Machine learning (ML) tools were employed to identify seven critical descriptors influencing  $D$  values: bond lengths (BL1, BL2, BL3), bond angles (BA1, BA2, BA3), and the parameter  $\phi$ . This dataset was shuffled and split, with 80% used for training and 20% for testing. The ML model achieved over 90% accuracy in  $D$  value prediction and over 95% in classification, offering a deeper understanding of the relationship between structural features and magnetic properties in SMMs.

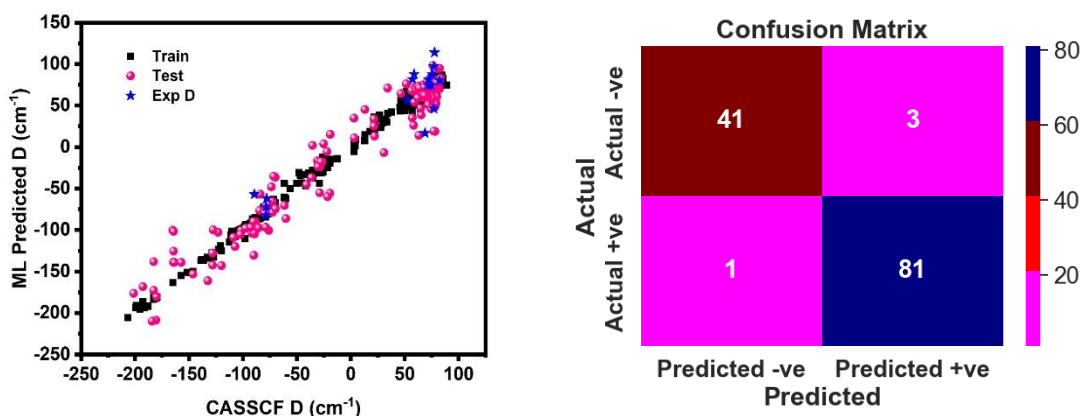


Figure 1. (a) Scatter plots illustrate the comparison between ML-predicted, CASSCF-calculated  $D$ , and experimentally reported values within both training and testing datasets. (b) Binary confusion matrix with an actual sign on the y-axis and predicted sign on the x-axis.

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# Investigating the Influence of Oriented External Electric Fields on Modulating Spin-Transition Temperatures in Fe(II) SCO Complexes: A Theoretical Perspective

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Spin-crossover complexes, valued for their bistability, are extensively studied due to their numerous potential applications. A primary challenge in this molecular class is identifying effective methods to adjust the spin-transition temperature, which frequently falls outside the desired temperature range. This typically necessitates intricate chemical design and synthesis or the use of stimuli such as light or pressure, each introducing its own set of challenges for integrating these molecules into end-user applications. In this work, we aim to address this challenge using an oriented external electric field (OEEF) as one stimulus to modulate the spin-transition temperatures. For this purpose, we have employed both periodic and non-periodic calculations on three well-characterized Fe(II) SCO complexes namely [Fe(phen)<sub>2</sub>(NCS)<sub>2</sub>] (**1**, phen = 1,10-phenanthroline), [Fe(bt)<sub>2</sub>(NCS)<sub>2</sub>] (**2**, bt = 2,2'-bi-2-thiazoline) and [Fe(py)<sub>2</sub>phen(NCS)<sub>2</sub>] (**3**, py = pyridine) possessing similar structural motif of {FeN<sub>4</sub>N'<sub>2</sub>}. To begin with, DFT calculations employing TPSSh functional were performed on complexes **1** to **3**, and the estimated low-spin (LS) and high-spin (HS) gaps are 24.6, 15.3 and 15.4 kJ/mol, and these are in the range expected for Fe(II) SCO complexes. In the next step, OEEF was applied in the molecule along the pseudo-C<sub>2</sub> axis that bisects two coordinated -NCS groups. Application of OEEF was found to increase the Fe-ligand bond length and found to affect the spin-transition at particular applied OEEF. While the HS state of **1** becomes the ground state at an applied field of 0.514 V/Å, the LS state lies at a higher energy of 1.3 kJmol<sup>-1</sup>. While the DFT computed T<sub>1/2</sub> for the optimised geometry of **1**, **2** and **3** were found to be 134.6 K, 159.9 K and 111.4 K respectively, at the applied field of 0.6425 V/Å T<sub>1/2</sub> increases up to 187.3 K, 211.0 K and 184.4 K respectively, unveiling hitherto unknown strategy to tune to the T<sub>1/2</sub> values. Further, calculations were performed with complex **1** adsorbing on the Au(111) surface. The formation of an Au–S bond during adsorption significantly stabilises the low-spin (LS) state, hindering the observation of spin-crossover (SCO) behaviour. Nonetheless, the application of OEEF reduces this gap and brings the T<sub>1/2</sub> value closer to the desired temperature. This offers a novel post-fabrication strategy for attaining SCO properties at the interface.

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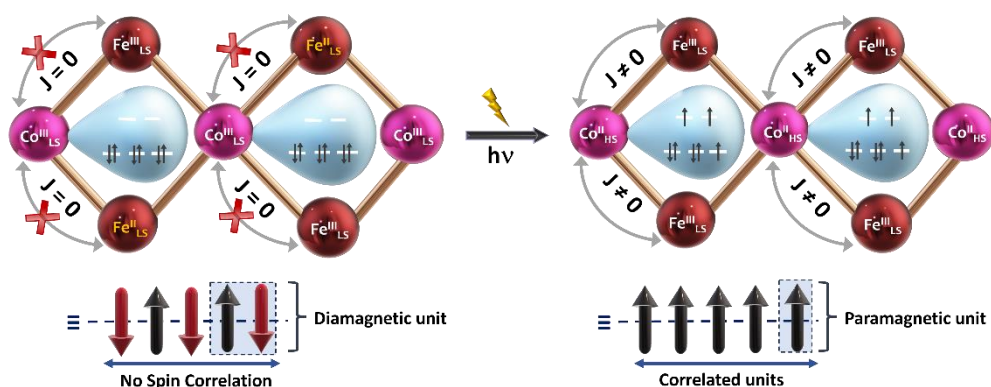
## Solvent Orchestrates Photo-responsive Behavior in cyanide bridged Fe<sub>2</sub>Co Single-Chain Magnet

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Single-chain magnets (SCMs) exhibit slow relaxation of magnetization, bistability, and hysteresis at the molecular level, making them promising candidates for next-generation switches, sensors, and storage devices.<sup>1</sup> The photo-switching of SCM behavior offers a pathway for prompt and contactless control of spin states and their associated properties. One strategy to achieve photo-responsive SCMs involves exploiting the photo-switchable electron transfer coupled spin transition (ETCST) in discrete cyanide bridged Fe-Co Prussian blue analogs (PBAs) by integrating them into a coordination polymer separated by suitable pendant or pillar ligands.<sup>2</sup> However, several factors like H-bonding,  $\pi$ - $\pi$  interactions, and CH- $\pi$  interactions can tune the ligand field strength and redox potential around the metal centers, stabilizing either  $\{\text{Fe}^{\text{II}}_{\text{LS}}(\mu\text{-CN})\text{Co}^{\text{III}}_{\text{LS}}(\mu\text{-NC})\text{Fe}^{\text{III}}_{\text{LS}}\}$  or  $\{\text{Fe}^{\text{III}}_{\text{LS}}(\mu\text{-CN})\text{Co}^{\text{II}}_{\text{HS}}(\mu\text{-NC})\text{Fe}^{\text{III}}_{\text{LS}}\}$  states, thereby ruling out the ETCST behavior.<sup>3</sup> The solvent, counterions, and guest molecules are known to participate in such interactions and thereby influence the ETCST behavior; hence, their choice during the synthesis of the molecule becomes inadvertently important. Our study on a 1D Fe<sub>2</sub>Co cyanide-bridged coordination polymer shows that solvent choice decides the fate of ETCST and photo-induced SCM behavior due to solvent-aided molecular packing and inter- and intra-molecular interactions, as will be discussed in the poster.

**Figure 1** Photo-induced ETCST leading to switching of the magnetic exchange interaction



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# Enhancing Spin-Transport Characteristics, Spin-Filtering Efficiency, and Negative Differential Resistance in Exchange-Coupled Dinuclear Co(II) Complexes for Molecular Spintronics Applications

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In this work employing an array of theoretical tools such as DFT, *ab initio* CASSCF/NEVPT2 method and DFT combined with NEGF formalism, we have studied in detail the role of magnetic coupling, ligand field and magnetic anisotropy in the transport characteristics of complex [Co<sub>2</sub>(L)(hfac)<sub>4</sub>] (**1**, Figure 1).<sup>1,2</sup> Particularly, our calculations not only reproduce the current-voltage (*I-V*) characteristics observed in experiments but also unequivocally establish that these arise from an exchange-coupled singlet state that arises due to antiferromagnetic coupling between two high-spin Co(II) centres. Further, the estimated spin Hamiltonian parameters such as *J*, *g* values, *D* and *E/D* values are only marginally altered for the molecule at the interface. The exchange-coupled state was found to have very similar transport responses, despite possessing significantly different geometries. Our transport calculations unveil a new feature of the negative differential resistance (NDR) effect on **1** at the bias voltage of 0.9 V, which agrees with the experimental *I-V* characteristics reported. The spin-filtering efficiency (*SFE*) computed for the spin-coupled states were found to be only marginal (~25%), however, if the ligand field is fine-tuned to obtain a low-spin Co(II) centre, a substantial *SFE* of 44% was noted. This spin-coupled state also yields a very strong NDR with a peak-to-valley ratio of ~56 - a record number that has not been witnessed so far in this class of compounds.

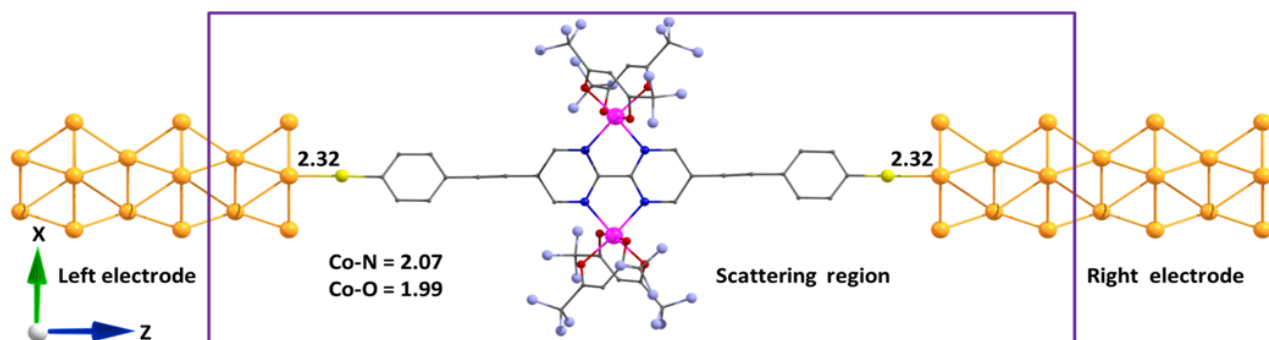


Figure 1. Molecular junction device of **1hshs**.

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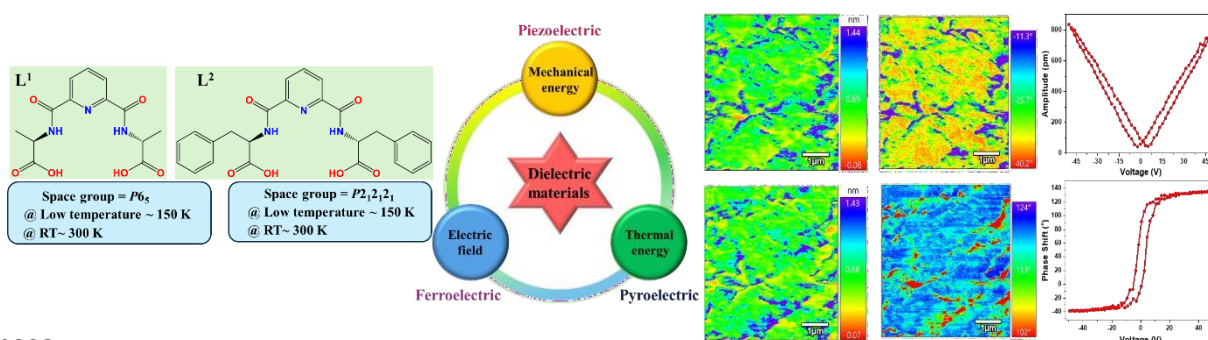
# Pyridine backboned di-peptide based metal free organic materials as piezoelectric energy harvesters

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The increasing demand for energy, driven by the explosion of electronic devices, along with the environmental concerns associated with traditional energy sources, has made renewable energy harvesting a top priority. Among the innovative solutions, piezoelectric energy harvesting through devices stands out for its ability to extract electrical energy from nearly all forms of mechanical energy met in numerous natural and artificial systems in daily life, such as physical movements, bending, pressing, and vibrations. Numerous devices utilizing conventional piezoelectric materials like lead zirconate titanate (PZT), ZnO, and BaTiO<sub>3</sub> had made for these specific applications which has their own limitations. Their poor mechanical flexibility, bio incompatibility, and ambient stability are key drawbacks, especially in areas such as wearable electronics, biomedical devices, or flexible sensors. To address these challenges, researchers are exploring alternatives such as organic and metal-free piezoelectric materials (like PVDF), polymer composites, and flexible nanomaterials, which offer enhanced mechanical flexibility and biocompatibility. Organic molecules with piezoelectric and ferroelectric properties have gained a wide interest for their applications in the domain of mechanical energy harvesting due to their desirable properties such as lightweight, thermal stability, mechanical flexibility, and ease of synthesis. Herein, we acquired pyridine backboned di-peptide based organic moieties-based acids (L<sup>1</sup> and L<sup>2</sup>) environmental benign materials as piezoelectric energy harvesting components. Pyridine-based ligands are generally chemically stable and soluble in wide ranges of organic solvents, making them easy to handle in synthetic applications. Not only pyridine-based dipeptide acids but their ester versions are also have been synthesized in bulk scales and we have extended the protocol toward the piezoelectric effect for those moieties. Using the slopes of the butterfly loop, the converse piezoelectric coefficient (d<sub>33</sub>) of these L<sup>1</sup> and L<sup>2</sup> were calculated around 20.51 ± 0.5 pm/V and 23.57 ± 0.5 pm/V, which are at par/higher than most of the conventional piezoelectric organic molecules. In addition, the work provides a detailed description of peptide-based piezoelectric materials as a bio-friendly alternative to current materials. These newer materials aim to overcome the limitations of traditional piezoelectrics while maintaining sufficient energy harvesting or sensing capabilities.



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## Tris-hydrazone ligand based C<sub>3</sub>-Symmetric trinuclear Ln-clusters in the perspective of Single-Molecule Toroids

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In recent days, Dy-based single-molecule magnets (SMMs) have become an emerging field for scientists due to their promising behavior to show a high anisotropic barrier for the reversal of magnetization as well as the high blocking temperature. To date, the highest blocking temperature in the range of liquid nitrogen has been achieved by a Dy-based SMM<sup>1</sup>. Along with this property of higher blocking temperature, C<sub>3</sub>-symmetric Dy<sub>3</sub>-clusters display a unique property called toroidal magnetic moment. A toroidal system shows a diamagnetic ground spin state and the magnetic property arises from the first excited state. This type of system can be used as quantum qubits in spintronic devices<sup>2,3</sup>. Keeping the focus on toroidicity, we have successfully synthesized two trinuclear Ln<sub>3</sub> [Ln=Dy and Yb] clusters [Ln<sup>III</sup><sub>3</sub>(H<sub>3</sub>ptk(bhz))<sub>2</sub>(CH<sub>3</sub>OH)<sub>6</sub>].3Cl·CH<sub>3</sub>OH [Ln=Dy(1), Yb(2)] [H<sub>3</sub>ptk(bhz)=N',N''',N''''-((1E,1E',1E'')-(2,4,6-trihydroxybenzene-1,3,5-triyl)-tris-(ethan-1-yl-1-ylidene))-tri-(benzohydrazide)] based on a tris hydrazone ligand. The primary characterization such as FT-IR, UV, SCXRD, PXRD, EDX, and TGA have been done for the systems.

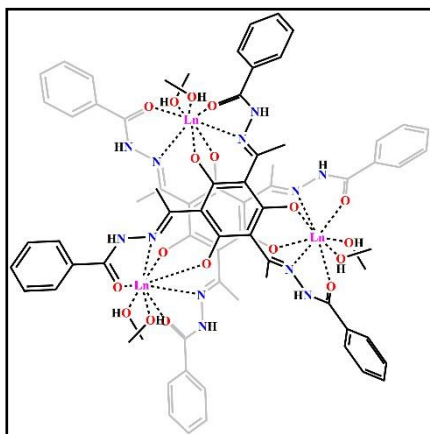


Figure 1: Chemical structure of the complexes

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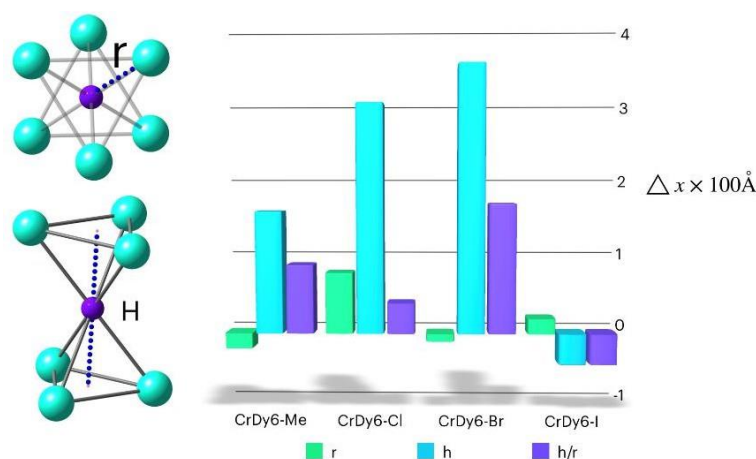
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# Fine-Tuning the FT-AFT Gap in {CrDy<sub>6</sub>} Complex through Electron Donating and Withdrawing Group Effects: A Combined Experimental and Theoretical Approach

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Toroidal states hold great promise for spin qubits, magnetoelectric coupling, spintronics, quantum sensing, etc, but stabilizing them at the molecular level remains challenging<sup>1,2</sup>. Enhancing toroidal moments requires long-range vortex ordering or sufficient dipolar coupling to control magnetic anisotropy. In our recent work, we studied {ML<sub>n</sub>6} complexes and found, for the first time, a ferrotoroidal ground state in a molecule. Compared to ferrotoroidal (FT) states, other states must be much higher in energy, ensuring a large FT- AFT (antiferrotoroidal) gap for application<sup>3</sup>. However, no known chemical strategies exist to increase this gap. We introduced Cl, Br, I, and CH<sub>3</sub> groups at the para position of the parent ligand (o-toluic acid) in similar structures to explore how electron-donating and withdrawing groups affect this gap<sup>4</sup>. Direct current (DC) magnetic measurements and theoretical calculations (RASSCF/RASSI\_SO/SINGLE\_ANISO/POLY\_ANISO) demonstrated that as the height-to-radius (h/r) ratio decreases, inter-triangle dipolar coupling units strengthen, leading to an increase in the FT-AFT gap.



**Figure 1.** The r, h, h/r - ratio of substitute {X-CrDy<sub>6</sub>} ( X = Me, Cl, Br, I ) relative to reported {CrDy<sub>6</sub>}

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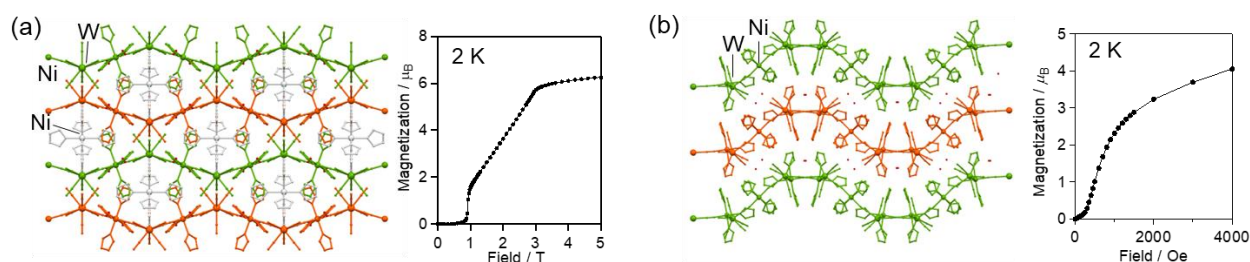
## Metamagnetic properties in two types of Ni-W cyanide assemblies

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Cyanide-bridged bimetal assemblies are molecule-based magnets that exhibit various magnetic functionalities, including photomagnetism. In this work, we present two types of cyanide-bridged Ni-W magnets:  

$$[\text{Ni}^{\text{II}}(\text{imidazole})_6]\{[\text{Ni}^{\text{II}}(\text{imidazole})_4][\text{W}^{\text{V}}(\text{CN})_8]\}_2 \cdot 4\text{H}_2\text{O} \quad (1),$$

$$[\text{Ni}^{\text{II}}(\text{pyrazole})_4]\{[\text{Ni}^{\text{II}}(\text{pyrazole})_3][\text{W}^{\text{V}}(\text{CN})_8]\}_2 \cdot 3.5\text{H}_2\text{O} \quad (2).$$
 Single crystals of 1 and 2 were prepared by mixing aqueous solutions of  $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ ,  $\text{Cs}_3[\text{W}(\text{CN})_8] \cdot 2\text{H}_2\text{O}$  and imidazole or pyrazole. Crystal structures were determined by SC-XRD. Magnetic properties were measured by SQUID magnetometer. SC-XRD revealed that 1 has a monoclinic structure (C2/m). 1 consists of one-dimensional anionic zigzag chains of  $\{[\text{Ni}^{\text{II}}(\text{imidazole})_4][\text{W}^{\text{V}}(\text{CN})_8]\}_n^{n-}$  and isolated counter cations  $[\text{Ni}^{\text{II}}(\text{imidazole})_6]^{2+}$  (Fig. 1 a). Magnetic studies indicated 1 exhibited a spin-flop transition at under an external magnetic field of 0.95 T (Fig. 1 a). Compound 2 was found to have an orthorhombic structure (Pbcn), consisting of a two-dimensional layered cyano-bridged Ni-W framework (Fig. 1 b). This compound exhibits spontaneous magnetization below 21 K, with interlayer antiferromagnetic interactions. These interlayer interactions were overcome by an external magnetic field of 400 Oe at 2 K, resulting in a spin-flip transition (Fig. 1 b).



**Figure 1** (a) Crystal structure of and MH curve of **1**, (b) crystal structure and MH curve of **2**.

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## Ferromagnetism in Porphyrinic Based 2D Sheets

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Magnetism in two-dimensional sheets has gained increased attention due to its promise for a variety of applications in magnonics<sup>1</sup>. Since graphene is non-magnetic, alternate structures like porphyrin based microstructures<sup>2</sup> provide an effective alternative for non-metal ferromagnets<sup>3</sup>. Here we designed a carbon-nitrogen network of benzo bisimidazole units that exclusively create a porphyrinic cavity when extended into a 2D sheet (Figure 1). Since porphyrin is a non-innocent ligand having an aromatic macrocycle known for nearly degenerate HOMO and HOMO-1 ( $a_{1u}$  and  $a_{2u}$ ) resembling simple aromatic rings, we show that oxidation to a neutral state stabilizes the quintet by  $\sim 3$  kcal/mol and a narrow spin-flip band gap; its geometry shows slight bond-alternation due to oxidation.

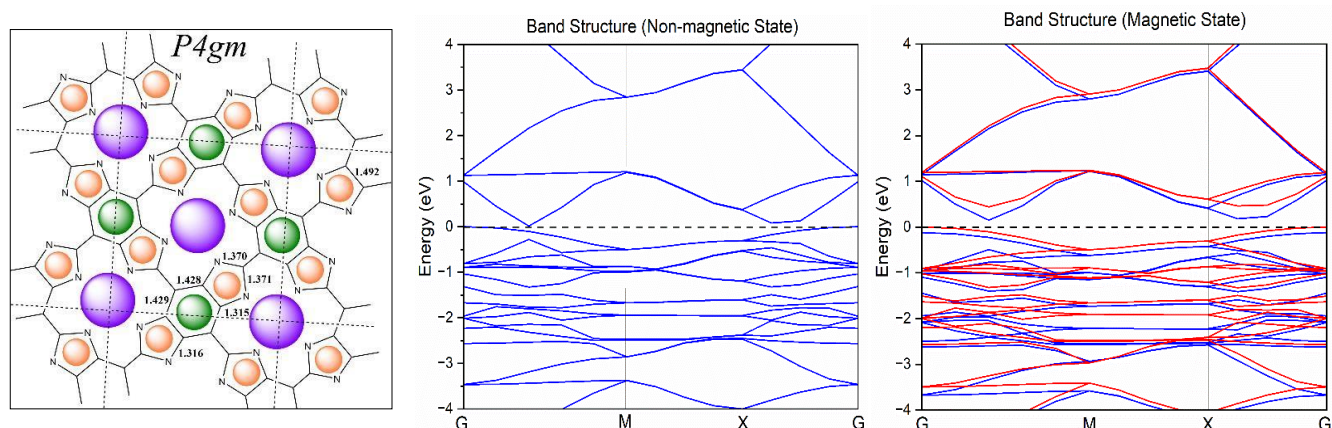


Figure 1: Structure of the DFT optimized Ferromagnetic unit cell of C<sub>2</sub>N (Z=8) 2D network (left), its non-spin polarized (middle) and Ferromagnetic (right) band structures.

The spin density is found to be extensively delocalized over the entire skeleton and causes mild bond alternation in the network. The band gap of non-magnetic phase (Figure 1b), is increased slightly in its ferromagnetic phase (Figure 1c).

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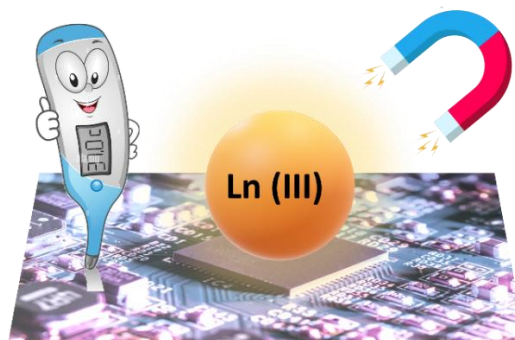


## The effect of conjugation in tuning the SMM and luminescence thermometry of two di-nuclear lanthanide complexes

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Effective control and detection of temperature are vital for optimizing the performance of molecular-based magnets.<sup>1</sup> Traditional direct contact methods are inadequate for detecting temperature in single molecular magnets (SMMs). Therefore, an appropriate thermometer that can monitor heat without interfering with the system is essential. Combining single-molecule magnets with luminescent properties in the same complex will aid researchers in understanding the mechanisms of heat generation in devices and allow for temperature monitoring at the submicrometer scale without disrupting the system.<sup>2</sup> Although, achieving an enhanced single-molecule magnet (SMM) along with luminescence in the same molecule is challenging, as SMMs typically require a high-symmetry point group, while luminescent properties necessitate a lower symmetry.<sup>3</sup> These two requirements are often incompatible. However, the essential factor that connects these two properties is emphasized here: the rigidity imparted by extended conjugation in the ligand backbone. Herein, we have synthesized two dinuclear dysprosium complexes with varying levels of ligand conjugation, and their SMM and variable temperature luminescence behavior have been analyzed. The complex bearing more conjugated ligands demonstrates enhanced SMM performance and improved luminescence thermometry. Rigidity minimizes phonon-mediated Raman contributions, thereby enhancing the single-molecule magnet (SMM) performance. Additionally, by decreasing vibrational relaxation, it increases the efficiency of ligand sensitization, thereby resulting in improved luminescence intensity of the complex.



**Figure 1** Schematic representation of the integration of SMM and luminescence thermometry in Dy (III) complex for opto-magnetic devices.

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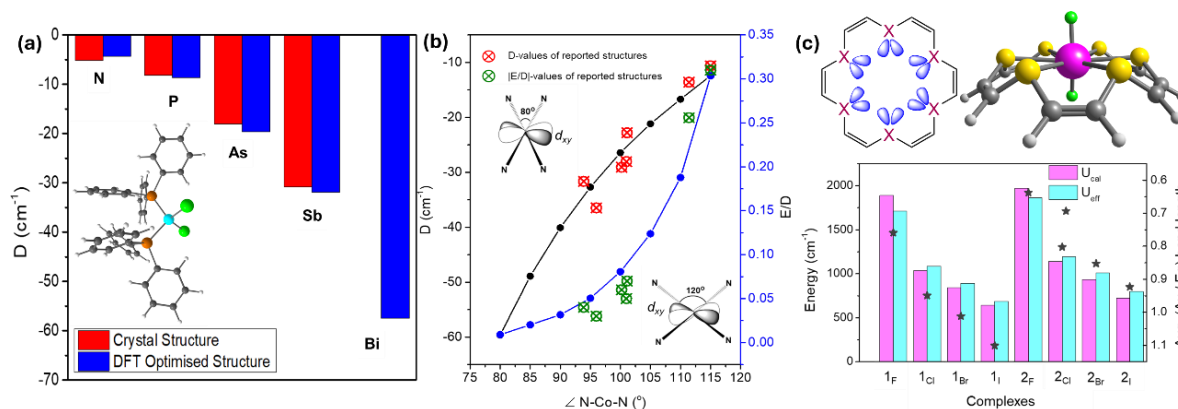
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## Computational Insights into Modulating Magnetic Anisotropy in Mononuclear Single-Molecule Magnets

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In the quest to find new Single Molecule Magnets (SMMs), one of the key factors for slow relaxation of magnetization is the magnetic anisotropy. Structural modifications, particularly in transition metal and lanthanide based mononuclear complexes, can significantly influence magnetic anisotropy. Another key strategy involves introducing heavy atoms into the ligand environment to enhance spin-orbit coupling and metal-ligand covalency.<sup>1–4</sup> Our study first examines Co(II) tetrahedral complexes using ab-initio methods to evaluate the effects of ligand modifications on magnetic anisotropy. We vary the donor atom from nitrogen to bismuth in  $\text{Co}(\text{ER}_2)_2$  molecules and investigate structural distortions using  $[\text{Co}(\text{pdms})_2]^{2-}$  with varying bite angles of the N-Co-N bond. The second part explores Dy(III)-based unsaturated 18C6 crown complexes in hexagonal bipyramidal environments. We study  $[\text{C}_{12}\text{H}_{12}\text{E}_6]$  (E = O, S, Se) rings as equatorial ligands and halides (F, Cl, Br, I) as axial ligands. These investigations aim to reveal the factors influencing magnetic properties in these systems, guiding the design of future SMMs.<sup>5,6</sup>



**Figure 1:** (a) Variation in D-value with inclusion of heavy atom in Co(II) complexes; (b) Correlation between the bite angle and the D-value; (c) Effect of ligand modulation in hexagonal bipyramidal Dy(III) complexes

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## Modulating Magnetic Anisotropy and Luminescence in Lanthanide Complexes and its Application as SMM Transistor

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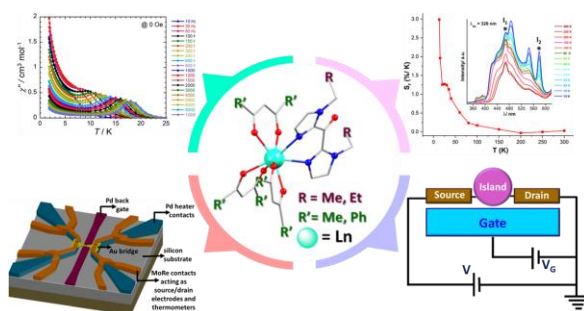
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Lanthanides have attracted attention in the field of Single Molecule Magnets (SMMs) since they have high spin-orbit coupling constant and high ground state spin, thereby leading to high magnetic anisotropy and enhanced effective energy barrier. The temperature dependence of the luminescence property of these Lanthanide complexes gives them an additional property of *in-situ* temperature monitoring, thereby leading to multifunctionality.<sup>1, 2</sup> We have prepared mononuclear, air-stable systems, of which, in this poster, I will be discussing the magnetic and optical properties of the Dy, Nd and Ho analogues.<sup>3</sup> The Dy and Ho analogues showed SMM like behaviour at 0 Oe applied DC field and the Nd complex shows field-induced SMM behaviour at 1500 Oe. The intrinsic luminescent properties of the 4f elements were also explored for luminescent thermometric application.<sup>3</sup> We have tried the single-molecule conductance measurements with [Dy(acac)<sub>3</sub>bik-Et] at the molecular junctions (MJs) in collaboration with Prof. Herre van der Zant at TU Delft. The system exhibited multiple configurational changes, revealing features indicative of a SMM.<sup>4, 5</sup>



**Figure 1** – Schematic presentation of the Lanthanide complexes and its salient properties.

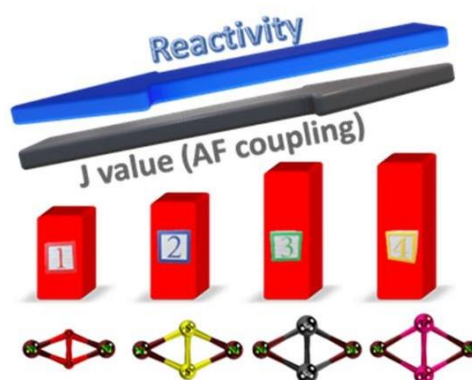
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# Role of Coupling Strength, Cooperativity, and Covalency Dictating the C–H Bond Activation Reactivity in Ni<sub>2</sub>E<sub>2</sub> (E = O, S, Se, and Te) Complexes

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Dinickel dichalcogenide complexes are critical for catalysis, electron transfer, magnetism, materials science, and energy conversion, with their structure and reactivity being key factors in these applications. These complexes are categorized as dichalcogenide or subchalcogenide based on metal oxidation<sup>1,2</sup> and the coordinated chalcogen, though their classification can be ambiguous due to complex electronic structures. Using DFT, CASSCF/NEVPT2, and DLPNO-CCSD(T) methods, we studied [(NiL)<sub>2</sub>(E<sub>2</sub>)] (E = O, S, Se, Te)<sup>3</sup> complexes and explored their reactivity toward C–H bond activation. Our results reveal a reactivity trend of {Ni<sub>2</sub>O<sub>2</sub>} > {Ni<sub>2</sub>S<sub>2</sub>} > {Ni<sub>2</sub>Se<sub>2</sub>} > {Ni<sub>2</sub>Te<sub>2</sub>}, driven by differences in Ni–E bondcovalency and electronic cooperativity between Ni centers, which shift their classification during reactions. Additionally, non-adiabatic analysis shows a decrease in coupling strengthdown the the group, indicating a relationship between metal-ligand covalency and reactivity. The reactivity trend correlates with the antiferromagnetic exchange coupling constant J, and our magneto-structural-barrier map offers a new way to fine-tune the reactivity of these complexes.



**Figure 1** Coupling strength correlation with catalytic reactivity for all four complexes.

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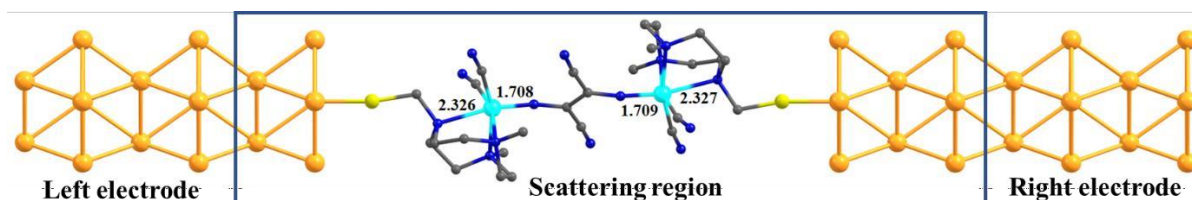
# Exploring Spin Transport Characteristics of Mixed-Valence $\{V^{IV}-V^{III}\}$ Magnetic Dimer: Probing the Interplay of Magnetic-Exchange and Double-Exchange Effects

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This study delves into the exploration of coherent transport properties of single-molecule junction (SMJ – Figure 1) devices featuring the molecule  $[(Me_3tacn)_2V_2(CN)_4(\mu-C_4N_4)]$  (**1**).<sup>1,2</sup> Employing a combination of DFT, ab initio CASSCF/NEVPT2 and NEGF calculations, we explored the spin state energetics, magnetic properties, and quantum transport characteristics of these complexes, aiming to uncover their potential applications in molecular spintronics devices.<sup>3-6</sup> The complex **1**, upon one-electron reduction (**1<sub>red</sub>**), exhibited Robin-Day class III mixed-valence magnetic dimer characteristics. The neutral state displayed strong antiferromagnetic coupling, which switched to ferromagnetic upon reduction. DFT calculations revealed an antiferromagnetic exchange interaction of  $-97\text{ cm}^{-1}$  between the  $V^{IV}$  centres, consistent with the experimental reported value of  $-112\text{ cm}^{-1}$ . The TD-DFT calculations confirmed strong intervalence charge transfer in reduced state, making  $S = 3/2$  the ground state with the double-exchange parameter,  $B \gg J$ . Quantum transport studies showed greater conductance in the high-spin state ( $S_T = 1$ ) compared to the broken symmetry state ( $S_T = 0$ ) in **1**, attributed to the presence of  $\beta$ -empty states in the conduction band near Fermi energy. The **1<sub>red</sub>** exhibited an enhanced spin transport characteristics due to complete electron delocalization between the V centres.



**Figure 1.** SMJ device to compute the quantum transport properties through the complex **1<sub>red</sub>**.

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## Misfit Layered Nanotubes from $\text{La}_{1-x}\text{Y}_x\text{S-TaS}_2$ : Influence of Charge Transfer on Superconductivity and Charge Density Waves

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Nanotubes Misfit layered compounds (MLCs) hold a significant interest due to their charge transfer and structural properties. MLCs allow tuning the electronic structure/carrier densities of the hexagonal unit beyond the conventional electron doping by modulation of the chemical entity in the rocksalt unit. In the present work, we demonstrate synthesizing a series of nanotubes (NTs) from the quaternary misfit layered compound  $\text{Y}_x\text{La}_{1-x}\text{S-TaS}_2$  using a chemical vapor transport technique spanning the entire compositional range. The atomic structure and composition were established using ultrahigh-resolution electron microscopy, revealing a free-standing MLC superstructure with long-range structural ordering. Subsequent in-depth analysis shows in-phase substitution of La by Y in the LaS subsystem, leading to substantial modifications in the charge transfer properties and thereby, the density of states on  $\text{TaS}_2$ , when compared to pristine  $\text{LaS-TaS}_2$ . Further, this study explores the tunability of the plasmonic and vibrational properties within  $\text{Y}_x\text{La}_{1-x}\text{S-TaS}_2$ . The charge transfer characteristics revealed that Y effectively fills more electrons into Ta  $5d^2$  states than La, thereby substantially influencing the superconducting transition temperature and charge density waves. Density-functional theory calculations were employed to investigate the stability of  $\text{Y}_x\text{La}_{1-x}\text{S-TaS}_2$  across the entire compositional range to complement the experimental finding.



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## Role of Oxidation State on Anisotropy and the Spin-Phonon Relaxation in Single-Ion Magnets

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Almost three decades of continuous research in the field of Single molecular magnets has brought many laurels to the area. We have come a long way from discovering TbPc21 to achieving a blocking temperature of 80°C<sup>2</sup>, and things are moving very fast. All the efforts made in this direction are concerned with the ligand field improvement only. One important aspect that seems to be missed by most of us is the importance of metal ions in achieving anisotropy. In recent years, several bivalent lanthanide-based complexes have been made with almost all lanthanide ions starting from Ce to Lu<sup>3</sup>. Also, experimental and theoretical studies are done on these complexes to establish that these complexes show a far greater magnetic moment than their trivalent counterparts<sup>4</sup>. It leads to our enhanced interest in establishing the SMM properties in tetravalent lanthanide-based SMMs. Although tetravalent lanthanide complexes are not easy to synthesise, a number of Ce<sup>IV</sup> complexes have been studied in the past, and recently Tb<sup>IV</sup> complex was synthesized by Mazzanti and co-workers. Tetravalent lanthanide complexes will lead to more robust metal–ligand bonds, which will, in turn lead towards a large crystal field. As expected there is increase in the covalency of metal–ligand bond which is confirmed from DFT calculations. Theoretical studies based on CASSCF/RASSI-SO/SINGLE\_ANISO methods have played a prominent role in the design and development of molecular magnets. Particularly pioneering work related to the development of the relaxation mechanism for simple models such as Dy<sup>III</sup>-O, Dy<sup>III</sup>-(OH)<sub>2</sub> and Dy<sup>III</sup>-F helped experimentalists in the design of suitable ligand architecture leading to superior Dy SIMs.

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# Temperature induced kinematic effect: Jumping, splitting spinning and running of an organic salt crystal

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Dynamic crystals show salient behavior induced by external stimuli such as heat, light, pressure, mechanical force, humidity, pH, magnetic and electric field.<sup>1,2</sup> Properties of these crystals are used in actuators, sensors, optoelectronic devices, switches, smart mechanical devices, biomimetic devices and soft robotics etc.<sup>3</sup> The phenomenon of exhibiting mechanical effects like jumping, cracking, explosion, rolling, walking and wriggling in crystals upon varying temperature is referred as thermosalience.<sup>4</sup> Kinematic effect in thermosalient crystals is very rare.<sup>5,6</sup> Here we report kinematic effect of piperazinium-2, 3, 5, 6-tetrafluoroterephthalate salt (TFT-PPZ) crystal due to jumping, bursting, spinning and running motion at elevated temperature.

TFT-PPZ is a class III thermosalient compound.<sup>7</sup> The thermosalient behaviour of the crystal was first indicated in Differential Scanning Calorimetry (DSC) experiment (Fig.1a) and visualized in Hot stage microscopy (Fig.1c). DSC thermogram shows saw-tooth peaks from 150-180°C due to jumping and fragmentation of the crystals followed by a broad endotherm which may appear due to sublimation of the crystals. Hot-stage microscopy shows hopping of the crystals at above 150°C followed by bursting into smaller pieces. Subsequently these small pieces also show jumping. The crystal on the hot-stage at 200°C start spinning rapidly followed by running till these crystals completely sublimed from the hot-stage.

To rationalise the thermosalient behaviour Variable Temperature Single Crystal X-Ray Diffraction (VT-SCXRD) experiment were performed starting from 100K to 450K at 50K interval each. The crystal packing shows 2D layers formed by TFT and PPZ ions (Fig 1b) and the layers are stacked along b-axis. Analysis of VT-SCXRD data revealed biaxial negative thermal expansion (NTE) and uniaxial colossal positive thermal expansion (PTE) exhibited by TFT-PPZ with coefficient of thermal expansion (CTE) -47.0682, -7.7563, 228.4245 MK<sup>-1</sup> along the principal axes X1, X2 and X3 respectively (Fig 1d).

Jumping and bursting of crystals can be explained by anisotropic thermal expansion. However, spinning and running motion of the crystals can be attributed to sublimation of the crystals at elevated temperature.

Currently, we are doing quantitative analysis of the kinematic effect in the crystals of TFT-PPZ.

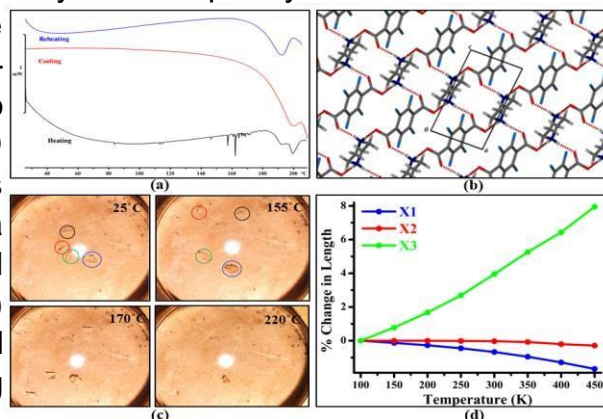


Figure 1. (a) DSC thermogram by heat-cool-heat method; (b) 2D layer formed by TFT and PPZ in the crystal structure viewed down b-axis; (c) Snapshot of hot-stage experiment showing the movement of crystals; (d) Thermal expansion of TFT-PPZ crystal

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## Role of Spin Crossover in Covalent Modification of AminoAcids in Cytochrome P460 Cofactor Maturation

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Post-translational modification (PTMs) in c-type cytochrome P460 through covalent cross-linking involves the heme porphyrin ring itself at meso-carbon with Lys amino acid of the protein.[1] The site-directed mutagenesis of Lys with Tyr or Leu does not cross-link and leads to catalytic inactivity for  $\text{NH}_2\text{OH}$  oxidation.[2,3] The origin of heme-Lys cross-link withleans of the functional and co-factor electronic structure remains elusive to date, and its study is highly demanding for mapping the artificial enzyme design. Specifically, the role of cross-link needs a virtuous theoretical prediction that has triggered the exciting advances inenzyme chemistry, particularly mechanistic insight.

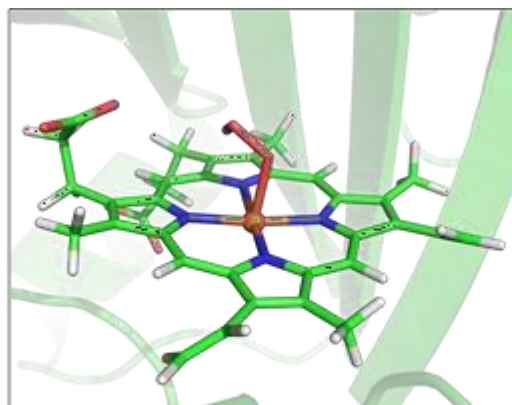


Figure 1: Active site for cyt P460 intermediate from *Nitrosomonas europaea*. PDB ID: 8GAR

To this extent, we have studied the dynamics and mechanism for maturation of cross-linkedcyt P460 as well as spectroscopic validation of intermediate observed by experimental studies using QM/MM calculation.

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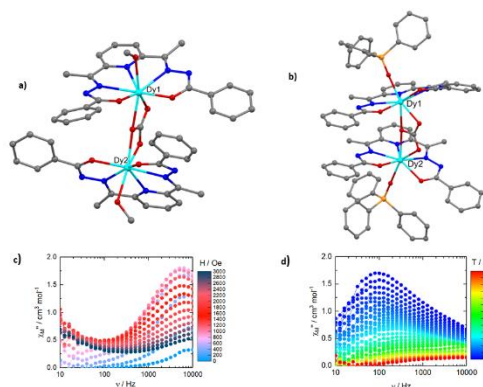
# Lanthanide Mediated Utilization of Aerial CO<sub>2</sub> Towards Designing Efficient Single Molecule Magnets

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Ever-growing CO<sub>2</sub> concentration in the atmosphere is one of the prime causes for the global climate change. It's an urgency to develop the strategies for efficient carbon capture. Chemical fixation and activation of CO<sub>2</sub> is regarded as the most effective strategy as it could lead to value-added products alongside the CO<sub>2</sub> removal from the atmosphere. Notably, lanthanide ions (Ln), especially trivalent dysprosium ion-based complexes, have exhibited fascinating single-molecule magnet (SMM) behavior.<sup>1</sup> Moreover, Ln ions are also realized for efficient fixation for CO<sub>2</sub>.<sup>2</sup>



**Figure 1:** The ball-and-stick models of the Dy analogues for the dinuclear complexes with crystallographically axially coordinated MeOH (a) and Ph<sub>3</sub>PO (b), the field-dependent *out-of-phase* ac susceptibility of the MeOH coordinated Dy analogue (c), and the temperature-dependent *out-of-phase* ac susceptibility of the Ph<sub>3</sub>PO coordinated Dy analogue (d). The H-atoms are omitted for clarity. Color codes: cyan, Dy; orange, P; red, O; blue, N; grey, C.

We will present the employment of Schiff base ligands with N<sub>3</sub>O<sub>2</sub> coordinating sites in complexation reactions with trivalent lanthanides. These reactions lead to the fixation of aerial CO<sub>2</sub> and the formation of carbonate-bridged dinuclear complexes (Figures 1a-1b). These complexes are found to be robust magnetic building blocks. Notably, post-synthetic modification (PSM) is believed to be extremely challenging, especially in the arena of Ln coordination chemistry. Nonetheless, it can be implemented on these dinuclear complexes. We will also exhibit how the SMM behavior of these dinuclear motifs could be tailored by tuning various ancillary ligands through the inner coordination PSM. For example, the Dy analogue of the dinuclear complexes with coordinated MeOH at the crystallographically axial sites is found to display field-induced SMM behavior (Figure 1c). The zero-field SMM behavior is switched on upon substituting these axial MeOH with triphenylphosphine oxides (Ph<sub>3</sub>PO, Figure 1d).

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## Unveiling the Local Atomic Structure of Cr-Implanted InGaO<sub>3</sub> Superlattices to Correlate with Infrared Emission Luminescence

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Battery-powered near-infrared (NIR) light sources are essential for modern technological applications such as spectroscopy, optical communication, anti-counterfeiting, night vision, and non-invasive medical diagnostics. NIR phosphor-converted LEDs (pc-LEDs), which use phosphors to convert high-energy light into lower-energy NIR light, are emerging as efficient, compact, and cost-effective alternatives to traditional infrared sources. Cr<sup>3+</sup> ions are preferred activators in NIR phosphor design due to the sensitivity of their outer d orbitals to local environments. However, the performance of Cr<sup>3+</sup>-based pc-LEDs strongly depends on the host crystal lattice, and challenges like trade-offs between spectral distribution and radiant power have limited their industrial applications. We recently introduced a design strategy utilizing edge-shared octahedral dimers to form stronger exchange-coupled Cr<sup>3+</sup>-Cr<sup>3+</sup> ion pairs ( ${}^2E \rightarrow {}^4A_2$ ), which led to broadband NIR emission with zero thermal quenching. Additionally, Cr<sup>3+</sup> clustered luminescence ( ${}^4T_2 \rightarrow {}^4A_2$ ) was achieved by utilizing long chains of edge-shared octahedral dimers in intermediate spinel structures, resulting in near-unity quantum efficiency and uniform spectral distribution. However, challenges persist in understanding the electronic transition behaviour ( ${}^2E \rightarrow {}^4A_2$  and  ${}^4T_2 \rightarrow {}^4A_2$ ) and the origins of these phenomena, as traditional Tanabe-Sugano diagrams are limited in explaining these transitions. To better understand the structure-luminescence relationship of Cr<sup>3+</sup> ion pairs and clusters, studying them in simple host lattices with varying coordination geometries is important. In this context, we explore the In<sub>1-x</sub>Cr<sub>x</sub>GaO<sub>3</sub> series as phosphors, featuring Cr<sup>3+</sup>-Cr<sup>3+</sup> ion pair emission in the NIR range of 650–1000 nm. Stronger shortwave near-infrared (SWIR) emissions in the 1200–1600 nm range were observed for  $x > 0.07$ . We evaluate the origin of the Cr<sup>3+</sup>-Cr<sup>3+</sup> ion pair and SWIR emissions by obtaining complete structural information through Rietveld refinement and XAS techniques. This study provides detailed insights into the formation of Cr<sup>3+</sup>-Cr<sup>3+</sup> ion pairs, offering guidance for the future design of phosphors that achieve broader near-infrared emission without the need for additional activators or co-dopants, thereby improving performance.



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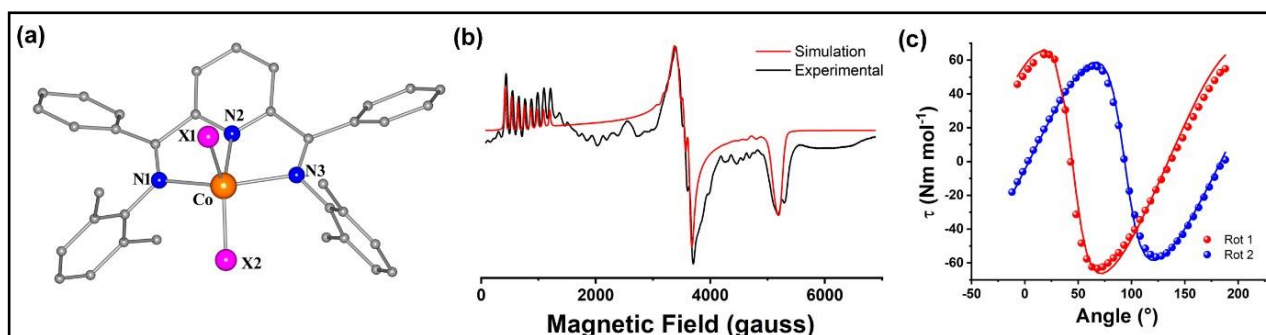
# Quantifying Magnetic Anisotropy of Series of Five-coordinate Co<sup>II</sup> ions: Experimental and Theoretical Insights

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Stabilizing large easy axis type magnetic anisotropy in molecular complexes is an extremely challenging task, yet it is crucial for the development of molecular-based information storage devices and its applications in molecular spintronics. Achieving this requires a profound understanding of electronic structure and the relationships between structure and properties, to develop magneto-structural correlations. Herein, we report a series of five-coordinate distorted square pyramidal Co<sup>II</sup> complexes [Co(L)(X<sub>2</sub>)]·CHCl<sub>3</sub> (where X = Cl(**1**), Br(**2**), or I(**3**)), all exhibiting axial anisotropy (D). The D was quantitatively determined for all members of the series (**1** = -72; **2** = -67 and **3** = -25 cm<sup>-1</sup>) using a high-precision Cantilever Torque Magnetometer (CTM) which is firmly supported by magnetic susceptibility, and EPR measurements. The study of the magnetization relaxation dynamics reveals the presence of field-induced slow relaxation of magnetization. Theoretical calculations on **1-3** and certain model complexes shed not only the electronic structure but also provide the influence of steric and electronic effects in modulating the D values. Overall, these studies open new avenues for designing next-generation Co<sup>II</sup> complexes with improved D values and a reduced |E/D| ratio.



**Figure 1:** (a) Representative molecular structure of complex **1-3**. Solvent moiety and hydrogen atoms are omitted for clarity (b) X-band EPR spectrum of magnetically diluted **2-dil** at 5.0 K (c) Torque signals for **2** at 2.0 K and in a magnetic field of 4 T. The solid lines are the best-fit curves for Rotation 1 and 2.

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## “Exploring the magnetic behavior of $\{Ln_2\}$ Single Molecule Magnets with diverse bridging ligands. Synthesis and theoretical Insights.”

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The magnetic properties of dinuclear lanthanide complexes arise from the interaction between the two lanthanide centers. This can lead to cooperative effects that influence the overall magnetic behavior of SMMs. Various factors influence these system's energy barriers, but the major is Magnetic Exchange Interactions.<sup>[1]</sup> The geometry of the dimer, including the spatial arrangement of the magnetic centers and the nature of the bridging ligands, significantly impacts the magnetic properties.<sup>[2]</sup> We have successfully synthesized paddle-wheel type geometry of  $\{Ln_2\}$  complexes with the formula  $[Ln_2(C_6F_5COO^-)_6(H_2O)_2(bpy)_2]$  ( $Ln = Tb$  (1),  $Dy$  (2),  $Ho$  (3), and  $Er$  (4)), allowing for strong magnetic exchange interactions between the lanthanide ions. These interaction's nature and strength significantly impact the dinuclear complexes' overall magnetic properties with carboxylate ions acting as the bridge. Also, we selected seven parent dihalogen-bridged complexes with four different halogen bridges i.e.  $F^-$ ,  $Cl^-$ ,  $Br^-$ , and  $I^-$ , and performed *ab initio* calculations on the same. And then replaced the halogen of each parent complex with the remaining halogens. The studies are expected to reveal how the nature of the halogen bridge affects the magnetic interactions between the lanthanide ions transmitted, thereby influencing the overall anisotropy.

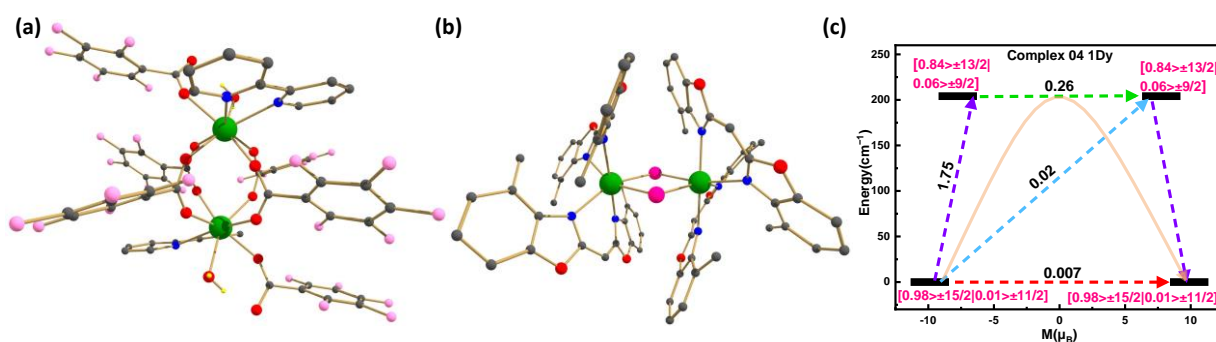


Figure 1: Structure of dinuclear (a)  $\{Dy_2\}$  complex, (b) reported  $\{Dy_2Cl_2\}$ <sup>[3]</sup> complex, (c) *ab initio* computed energy barrier for one of the Dy(III) ion of  $\{Dy_2Cl_2\}$ .

### References:

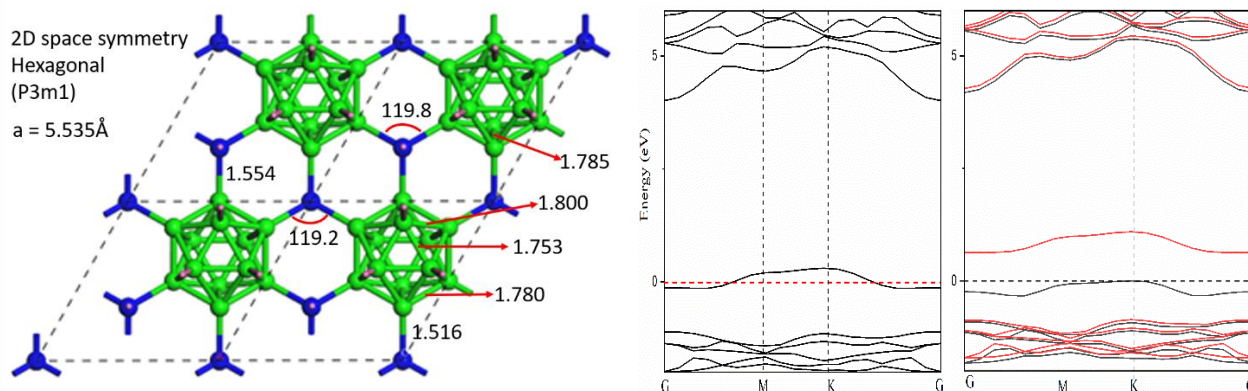
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## Metal-Free Ferromagnetism in B<sub>12</sub> based 2D sheets: Oxidation Induced by Electronegative Bridges

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Magnets of sp-elements are expected to have stiff spin-waves<sup>1</sup>, as their magnons exhibit stoner ferromagnetism with a high curie temperature, promising for spintronics and quantum information processing. Icosahedral B<sub>12</sub> has been proven to undergo facile oxidation when substituted with non-metals in molecules<sup>2</sup> and borides<sup>4</sup>. Though electron-deficient B<sub>12</sub>-based 3D networks are rigid, they show a non-magnetic ground state. Here, we show that the hexagonal (rhombohedral) borides with electronegative bridging atoms prefer a ferromagnetic state when their dimensionality is reduced to 2D.



**Figure 1** Structure of the DFT optimized (a) Ferromagnetic unit cell of (B<sub>12</sub>H<sub>6</sub>)(N)(NH) 2D network, its (b) non-spin polarized and (c) Ferromagnetic band structures.

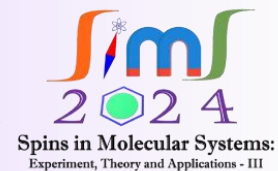
Our DFT calculations (GGA-PBE/otfg ultrasoft pseudo potentials @ 530 eV plane wave cut-off) show that the spin-polarized phase is stabilized by ~3 kcal per B<sub>12</sub> unit for various non-metal bridges. The bridging atoms planarize to aid delocalization, as illustrated in the (B<sub>12</sub>H<sub>6</sub>)(N)(NH) network shown in Figure 1a. Unlike the metallic non-magnetic phase (Figure 1b), its ferromagnetic phase has an indirect band gap of ~0.629 eV (Figure 1c).

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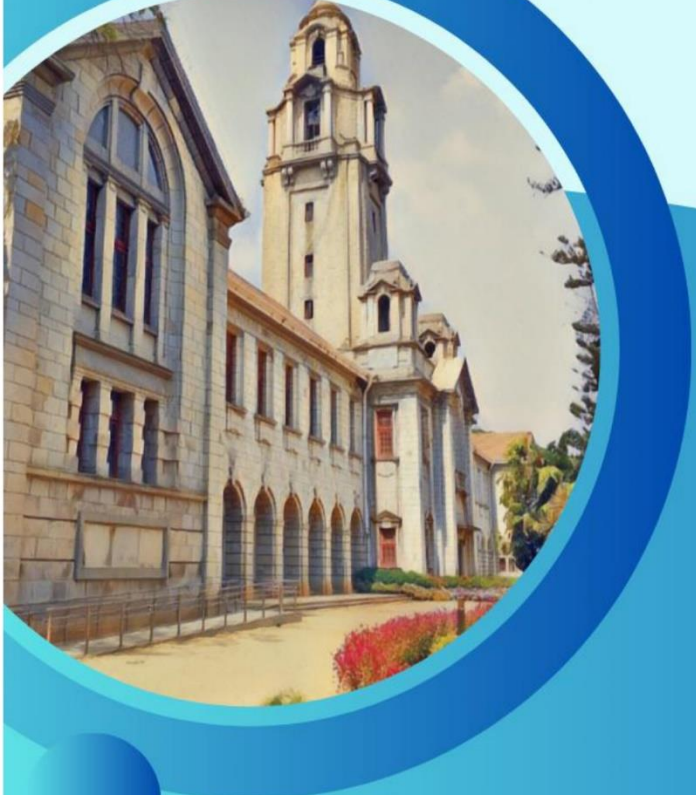
MODERN TRENDS IN MOLECULAR MAGNETISM – IV  
&  
SPINS IN MOLECULAR SYSTEMS:  
EXPERIMENT, THEORY AND APPLICATIONS – III



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# HORIBA

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The HORIBA Group headquartered in Kyoto, Japan, provides an extensive array of instruments and systems for applications ranging from automotive R&D, process and environmental monitoring, in-vitro medical diagnostics, semiconductor manufacturing and metrology.

HORIBA is a world leader in OEM Spectroscopy, Elemental Analysis, Fluorescence, Forensics, Particle Characterization, Raman, Ellipsometer, as well as XRF.

<p><b>Defect/Impurity Monitoring</b></p>  <p>LabRAM Soleil™</p>	<p><b>Emission Analysis</b></p>  <p>Duetta</p>	<p><b>Particle Characterization</b></p>  <p>Partica LA-960V2</p>	<p><b>Fluorescence Spectroscopy</b></p>  <p>FluoroMax-4 series</p>
<p><b>Raman Spectroscopy</b></p>  <p>XploRA Nano</p>	<p><b>Raman Spectroscopy</b></p>  <p>LabRAM Odyssey</p>	<p><b>Surface Analysis</b></p>  <p>GD-Profilor 2™</p>	<p><b>Thin Film Analysis</b></p>  <p>UVISEL Plus</p>
<p><b>Mass Flow Controller and Module</b></p>  <p>D700uF</p>	<p><b>Liquid Precursor Vaporizer</b></p>  <p>MV-2000</p>	<p><b>Pressure Controller</b></p>  <p>GR-511F</p>	<p><b>Vacuum and Gas Monitoring</b></p>  <p>Micropole System QL Series, IR-400, VG-200S</p>
<p><b>Plasma Monitor and Controller</b></p>  <p>EV 2.0 Series</p>	<p><b>Non-Contact Temperature Measurement</b></p>  <p>IT-270</p>	<p><b>Particle Detection</b></p>  <p>PD Xpation</p>	<p><b>Particle Analysis</b></p>  <p>Partica CENTRIFUGE CN-300</p>

Contact us at:

**HORIBA India Pvt. Ltd.**

246, Okhla Industrial Estate Phase III, New Delhi - 110020, India, Tel: +91 (11) 4646 5000 / 4669 5001, Email: marketing-ms.hin@horiba.com

Explore the future

**HORIBA**



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### S700X SQUID Magnetometer

Re-condensing cryostat with integrated VTI and high homogeneity magnet (R-S700X).

- No liquid helium refills
- No liquid Nitrogen.
- 1 Watt Pulse Tube cryocooler for true Zero boil-off system.
- Requires a 7.0 kW compressor which is water cooled
- Sample sits in liquid helium

Liquid Helium Cryostat with integrated VTI and high homogeneity magnet (S700X);

- 45 litre reservoirs for liquid helium and liquid nitrogen
- 2 to 4 litres per day of helium consumption.
- 5 litres per day liquid Nitrogen.

**Experts in Cryogen-free (CF) superconducting magnets for MR and EPR applications**

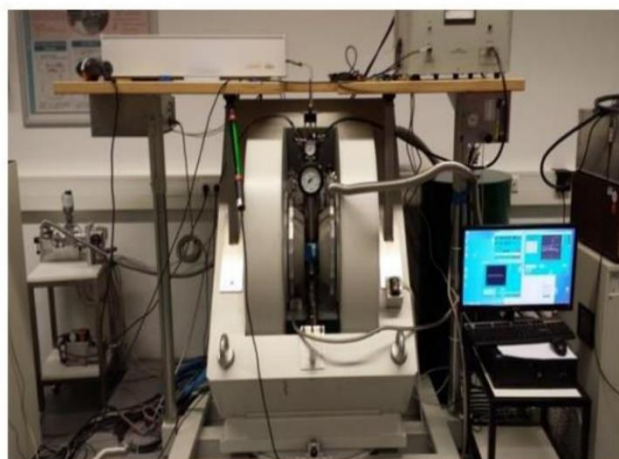
#### NMR

Cryogen free Wide/Narrow Bore magnet



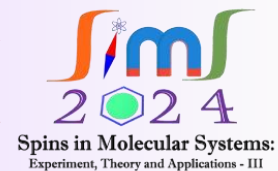
#### EPR

Cryogen free Variable Temperature Cryostat for Bruker spectrometer





**MODERN TRENDS IN MOLECULAR MAGNETISM – IV**  
**&**  
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**EXPERIMENT, THEORY AND APPLICATIONS – III**



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# LABMICRO MICROSCOPE



**SLV-61iFL**  
 Fluorescence Microscope



**SLV-21M**  
 Metallurgical Microscope




**SLV-22POL**  
 Polarizing Microscope



**SLV-23**  
 Research Microscope



**SLV-23 D**  
 Digital Microscope



**SLV-10M**  
 Student Microscope



**SLV-20i**  
 Laboratory Microscope



**SLV-40i**  
 Inverted Microscope



**SLV-53**  
 Digital Stereo Zoom Microscope

## Attachments



8 MP Camera  
 along with tab



Camera



Fluorescence



Micrometer Lens



Polarizing



Phase Contrast



- Elemental Analysis
- Raman Spectroscopic Analysis
- Water Quality Analysis
- Fluorescence/Cathodoluminescence Analysis

- Particle Characterization
- Surface Characterization
- Optical Components

# HORIBA

Your Partner in Science

## Analytical and Optical Solutions

.Research .Manufacturing .Recycling

Elemental Analysis			Particle Characterization		
<p><b>X-ray Analytical Microscope</b> <b>XGT-9000 Series</b></p>  <p>Next evolution of micro-X-ray fluorescence spectroscopy with ultimate performance in speed and flexibility for elemental imaging.</p> <p>QR Code: </p> <p>Detachable element: S, Si, Ar, Br, Cu, Fe, Ni, Pb, Pt, Zn                  Max. min. sample size: 300 x 250 x 60 mm (WxDxH)                  Maximum magnification: 120 x 100 mm                  (Sample chamber) Full vacuum, Part of vacuum</p>	<p><b>X-ray Fluorescence Analyzer</b> <b>MESA-50/MESA-50K</b></p>  <p>Desktop models for speedy elemental analysis of materials, with a sophisticated IN-line detector.</p> <p>QR Code: </p> <p>Detachable element: Al, Fe, Ni, S, Zn                  Spot size: 1.0 mm, 3.0 mm and 7 mm                  Dimensions: 298 x 294 x 235 mm (WxHxD)                  580 x 580 x 300 mm (MESA-50K) (W x D x H)                  Instrument weight: 12 kg (MESA-50)</p>	<p><b>X-ray Fluorescence Sulfur/Chlorine/Oil Analyzer</b> <b>MESA-7220V2</b></p>  <p>Measure ultra low sulfur and chlorine in petroleum products. Choose single position type or the 8-position transferable type.</p> <p>QR Code: </p> <p>Range: 0.00 – 100.00 ppm                  Detection limit: S: 0.7 ppm / Cl: 0.6 ppm                  (Certainty Standards) ASTM D4052 / D4059 / ISO 8254 / JIS K2217 / JIS K2221</p>	<p><b>Laser Scattering Particle Size Distribution Analyzer</b> <b>Partica LA-960V2</b></p>  <p>The system is known for its dynamic wide measurement range, excellent performance, ease of use and workable user-accepted quality.</p> <p>QR Code: </p> <p>Size range: 0.01 µm – 5,000 µm                  (Maximum particle size) 1 minute from disc on liquid filling and measurement to drying.                  (Optional accessories) Dry unit, MiniFlow unit, Fraction cell, Paste cell, etc. Please see the list below right.</p>	<p><b>Laser Scattering Particle Size Distribution Analyzer</b> <b>Partica mini LA-350</b></p>  <p>The compact Partica mini LA-350 can achieve high performance with easy operation and maintenance.</p> <p>QR Code: </p> <p>Size range: 0.1 µm – 1,000 µm                  (Dimensions) 267 x 420 x 378 mm (WxDxH)                  (Mass) Approx. 23 kg</p>	<p><b>Nano Particle Analyzer</b> <b>nanoPartica SZ-100V2 Series</b></p>  <p>This instrument analyzes three parameters that characterize nanoparticles: particle size, zeta potential and molecular weight.</p> <p>QR Code: </p> <p>Size range: 0.3 nm – 10 µm                  (Zeta potential) -500 – +500 mV                  (Molecular weight) 1 x 10<sup>3</sup> to 7 x 10<sup>6</sup> (kDa) (ppm)</p>
<p><b>X-ray Fluorescence Sulfur-in-Oil Analyzer</b> <b>SLFA-6100/6800</b></p>  <p>Compact and lightweight XRF sulfur-in-oil analyzer with excellent sensitivity and stability.</p> <p>QR Code: </p> <p>Range: 0 – 9.9999%                  Detection limit: 0.5 ppm or less                  (Certainty standards) ASTM D4054 / ISO 8254 / JIS K2541 / JIS K2542</p>	<p><b>X-ray Fluorescence Sulfur-in-Oil Analyzer</b> <b>SLFA-60</b></p>  <p>Compact and lightweight XRF sulfur-in-oil analyzer that provides easy and simple operation for petroleum products measurement.</p> <p>QR Code: </p> <p>Range: 0 – 9.9999%                  Detection limit: 0.5 ppm or less                  (Certainty standards) ASTM D4054 / ISO 8254 / JIS K2541 / JIS K2542</p>	<p><b>Sequential ICP Optical Emission Spectrometer</b> <b>Ultima Expert</b></p>  <p>Ultima Expert offers excellent resolution, low detection limits and full wavelength coverage optics for the most challenging applications.</p> <p>QR Code: </p> <p>(Total length) 100 cm                  (Spectral range) 120 – 820 nm                  (Resolution) 0.1 pm (P-AO) (0.1 nm) (A-SM) (0.05 nm)                  (Grating) 2,100 grooves / 1,320 grooves / 2,100 grooves (optional)</p>	<p><b>Centrifugal Nanoparticle Analyzer</b> <b>Partica CENTRIFUGE</b></p>  <p>High resolution particle size distribution measurement by centrifugation.</p> <p>QR Code: </p> <p>Size range: 10 nm – 40 µm                  (Flow centrifugal flow) 20,000 g                  (Temperature control) The rate, cell, and sample temperatures are controlled to a fixed temperature by the refrigeration.                  (Option) Density gradient (refractive) (DS501)</p>	<p style="text-align: center;"><b>Optional Accessories for Partica LA-960V2</b></p> <div style="display: flex; justify-content: space-around;"> <div style="width: 45%;"> <p><b>Imaging Analysis Unit (Built-in option)</b></p>  <p>Sample imaging can be observed with particle size distribution. Observation of aggregation, floccing material in sample.</p> </div> <div style="width: 45%;"> <p><b>High Concentration Cell</b></p>  <p>This accessory enables highly concentrated sampling. Some slurries and suspensions are already dispersed in certain conditioned liquids, therefore less dilution is required for particle size and distribution measurements.</p> </div> </div> <div style="display: flex; justify-content: space-around; margin-top: 20px;"> <div style="width: 45%;"> <p><b>MiniFlow (Circulation system)</b></p>  <p>Flow type measurement with 35 mL volume of dispersion medium is possible. It is recommended when using an organic solvent as a dispersion medium.</p> </div> <div style="width: 45%;"> <p><b>Fraction Cell</b></p>  <p>For minimal solvent requirements, such as ultra-trace amounts of sample, and when you want to recover the whole sample after measurement, it can measure from a minimum volume of 5 mL.</p> </div> </div> <div style="display: flex; justify-content: space-around; margin-top: 20px;"> <div style="width: 45%;"> <p><b>Dry Cell</b></p>  <p>Dry cell can can measure samples in a powder state. It supports both non-dispersive measurement with front fall and liquid dispersion measurement using compressed air.</p> </div> <div style="width: 45%;"> <p><b>Automatic Sampler (Wet measurement in powder)</b></p>  <p>The Auto Sampler is a rotary table-type automatic sampling system equipped with 24 diphasic sample cups.</p> </div> </div>	
<p><b>Oxygen/Nitrogen/Hydrogen Analyzer</b> <b>EMGA-Pro/Expert</b></p>  <p>High-speed measurements on oxygen, nitrogen and hydrogen content down to ppm level in metallic materials, such as steel products, non-ferrous alloys, electrical materials, etc.</p> <p>QR Code: </p> <p>(Method) Infrared Laser in hot gas, Non-Dispersive Infrared absorption measurement (ND), Thermal Conductivity Detector (TC)                  (Measurement range) Oxygen: 0.01 ppm – 5%                  Nitrogen: 0.01 ppm – 3%                  Hydrogen: 0.01 ppm – 2500 ppm                  (Accessories) Integrated auto-cleaner and or auto loader</p>	<p><b>Carbon/Sulfur Analyzer</b> <b>EMIA-Pro/Expert</b></p>  <p>Measures carbon and sulfur content down to ppm level in steel products, non-ferrous alloys, minerals, electronic materials and others, such as catalyst, rubber, etc.</p> <p>QR Code: </p> <p>(Method) Hot-heater type heating in oxygen stream for quantitative infrared absorption method                  (Measurement range) Carbon: 0.01 ppm – 10%                  Sulfur: 0.5 ppm – 1% (optional)                  (Accessories) Integrated auto-cleaner</p>	<p><b>Carbon/Sulfur Analyzer (or Temperature Rise Analysis)</b> <b>EMIA-Step</b></p>  <p>Measures carbon and sulfur content down to ppm level in steel products, non-ferrous alloys, minerals, electronic materials and the others, such as catalyst, rubber, etc.</p> <p>QR Code: </p> <p>(Method) Coulter electric resistance heating furnace type for quantitative infrared absorption method                  (Measurement range) Carbon: 0.01 ppm – 10%, Sulfur: 0.1 ppm – 1% (optional)</p>	<p><b>Nano Particle Tracking Analyzer</b> <b>ViewSizer 3000</b></p>  <p>Implements breakthrough improvements to particle imaging technology. It includes proprietary illumination and detection methods, allowing microscopic visualization measurement of a limited concentration of nanoparticles over a wide range of sizes.</p> <p>QR Code: </p> <p>(Measurement range) 10 nm – 15 µm                  (Typical sample volume) 100 µL – 1.5 mL                  (Dimensions) 520 x 600 x 500 mm (WxDxH)                  (Mass) 27 kg</p>		



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# MODERN TRENDS IN MOLECULAR MAGNETISM – IV

## &

# SPINS IN MOLECULAR SYSTEMS:

## EXPERIMENT, THEORY AND APPLICATIONS – III



### Raman Spectroscopic Analysis

#### Confocal Raman Imaging System LabRAM Soleil



Including state-of-art technologies and functions, perform even the most advanced research and highest confocal Raman imaging has never been so easy.



**Spectral range:** UV-Vis-NIR (200 - 1,600 nm) (Excitation source) Up to 4 parallel beams  
**Measurement function:** Ultra-deep (up to 100 (micrometer)) confocal imaging with parallel beam sharing function  
**Scan area:** 500 (micrometer) x 500 (micrometer) with 10x objective lens  
**Stage:** 6-axis under vacuum 30 cm<sup>3</sup>  
**Dimensions:** 808 x 797 x 808 mm (WxDxH)  
\*Compatible with our confocal Raman

#### Ultimate Raman Microscope LabRAM Odyssey



20+ PLD Raman measurement with high spatial resolution. Perfect for advanced materials and nanostructure studies with an optimized excitation from Deep UV to Infrared.



**Du-off:** <math>50\text{ cm}^3\text{ (Standard)}</math> <math><10\text{ cm}^3\text{ (Optional)}</math>  
**Spectral range:** 200 to 2,000 nm  
**Flexibility:** Up to 3 detectors and an unlimited number of beams (8 motorized)  
**Optional accessories:** Laser trapping, beam scan-beam accessories, Particle analysis software

#### Raman Microscope XploRA™ PLUS



Fully automated and fully confocal Raman microscope for fast, non-destructive chemical micro-analysis and Raman chemical imaging.



**Spectral range:** Visible light - Near-Infrared (530 to 1,120 nm) (Excitation source) Up to 4 (motorized) beams  
• Fast Raman imaging with SMT™ function  
• One-click operation

#### Affordable Benchtop Raman Spectrometer MacroRAM™



Brings simplicity to Raman measurements without compromising the ability to handle even complex samples, from extremely small liquid volumes to large solids. Its compact and robust design, including Class 1 laser safety, means it's safe for use in most environments. From undergraduate teaching labs to industrial QC applications.



#### Micro-Photoluminescence Spectrometer LabRAM Odyssey Semiconductor



Ideal for non-destructive, non-contact evaluation of compound semiconductor. It is the ideal tool for photoluminescence and Raman imaging on wafers up to 300 mm diameter.  
**Measuring wavelength range:** Ultraviolet - Red-Infrared (200 - 2,000 nm)  
**Sample temperature cells:** from 4 to 300K



#### Standard Microscope Spectroscopy Solutions Standard Microscope Spectroscopy



Take your add spectroscopy to any standard microscope for applications like: Photoluminescence (PL), Raman, Electrochromism (EC), Time-resolved PL (TRPL), and Dark Field Scattering Spectroscopy.



#### Optional Accessories for Raman Particle Disperser XD-100



Use for particles of dispersion in a simple and intuitive operation. Ideal sample preparation for challenging particle analysis with micro Raman, micro XRF, SEM or other microscopic techniques.



### Fluorescence/Cathodoluminescence Analysis

#### Fluorescence and Absorbance Spectrometer Duetta



Ultra fast, compact and two-in-one fluorescence and absorbance spectrometer for analytical molecular fingerprinting.



**Fluorescence detection range:** 250 - 1,100 nm (excitation) 300 nm - 1,000 nm (emission)  
**Absorbance detection range:** 190 - 1,000 nm (excitation) 250 - 999 nm (W-D-E-H) (emission) 250 - 999 nm

#### Benchtop Spectrofluorometer FluoroMax Plus



A compact benchtop instrument offering the ultimate in simplicity and flexibility. Dual detectors (UV-VIS and NIR) for wide range measurement.



**Light source:** 150 W CW xenon-arc or xenon (Optional excitation modes) Xenon arc (1,050 W, 100% duty cycle)  
**Photomultiplier**

#### Spectrofluorometer Nanolog

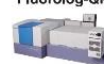


Supports fluorescence and photoluminescence measurements from UV to NIR regions and offers flexible system configuration for selecting specific ions.



**Wavelength range:** 200 - 850 nm (excitation) up to 2,000 nm (emission)  
**EM Range:** 16,000:1 (Raman scan in water, TSD)  
**Wavelength resolution:** 0.2 nm  
**Excitability:** emission lifetime, quantum yield, polarization, temperature control, etc.

#### Multichannel Fluorimeter for Lifetime and Steady State Measurements Fluorolog-QM



Offers all reflective optics, combined with a multitude of light source and detector options, and sample handling accessories, for the highest stability and versatility of any spectrofluorimeter.



#### Fluorescence Lifetime Spectrometer DeltaPro/DeltaFlex



DeltaPro/DeltaFlex are the next generation of time-correlated single photon counting (TCSPC) fluorescence lifetime instrumentation.



**Wavelength:** 650 nm (Laser) 700 nm - 650 nm (Excitation) 10.5 nm (nm) (Emission) 115 nm (Spectral range) 100 - 3000 cm<sup>-1</sup> (Resolution) 1000 - 1,700 cm<sup>-1</sup> (Spectral resolution) 6 cm<sup>-1</sup> at 212 nm (Spectral resolution) 7 cm<sup>-1</sup> at 832 nm (Spectral resolution)

#### SPM-Cathodoluminescence (CL) Spectral System CLUE Series



Provides high performance CL analysis for a wide range of applications for semiconductor, photovoltaic, and geology.



**Spectral range:** 140, 325, or 550 nm  
**Spectral range:** UV-Vis-NIR: 200 - 700 nm depending on configuration

### Optical Components

#### High Performance Compact Spectrometer MicroHR Series



A sleek, local long focal Chroma-Turner spectrometer that can be used as an imaging spectrograph or a scanning monochromator.



**Focal length:** 140 mm (Aperture) 0.88  
**Scanning range:** 10 - 1,000 nm mechanical range (motorized version)  
**Spectral dispersion:** 5.65 nm/mm at 600 nm

#### Imaging Spectrometer IHR320/550



Provides the most reliable optical solution with optimal solution for essential parameters in imaging spectrometers.



**Focal length (mm):** 320 (IHR320), 550 (IHR550)  
**Aperture:** f4.0 (IHR320), f6.4 (IHR550)  
**Spectral range:** 350 - 840 nm (at 1,200 g/mm grating)  
**Spectral dispersion:** 2.35 nm/mm at 450 nm, 1,200 g/mm (IHR320), 1.34 nm/mm at 485 nm, 1,200 g/mm (IHR550)

#### High Resolution Spectrometer FHR Series/M Series



These large focal length spectro meters are ideal for applications where extremely low stray light and high resolution are required, and offer a unique combination of high speed, precision and high spectral resolution.



**Focal length (mm):** 600 (FHR1000), 700 (FHR1200), 1,000 (FHR1500), 1,500 (FHR2000)  
**Aperture:** f5.4 (FHR1000), f6.0 (FHR1200), f6.0 (FHR1500), f5.0 (FHR2000)  
**Spectral resolution (nm/m):** 1.2 (FHR1000), 0.6 (FHR1200), 0.3 (FHR1500), 0.25 (FHR2000)

### Surface Characterization

#### Pulsed RF Glow Discharge Optical Emission Spectrometer (GD-OES) GD-Profiler 2



Fast, simultaneous depth profile analysis of elements. Ideal for multilayers and etched materials.



**Measurement range:** 1 (1) - 11 (9)  
**Scattering rate:** 1,000 (depending on sample)  
**Detector:** Standard, 15 ch, Maximum: 46 ch

#### Fully Automated Ellipsometer UVISEL Plus



Automated spectroscopic ellipsometer delivering excellent performance for nano and micro layer characterization.



**Spectral range:** 190 - 895 nm (UV extension) up to 2,100 nm  
**Spot size (in mm):** 10.25 - 0.1 (1 mm manual) 0.25, 0.32, 0.25, 1.2 mm auto-rotate (Angle range) 5° - 95° by steps of 5° manual, 45° - 95° by steps of 0.1° auto-rotate

### Water Quality Analysis

#### pH / Water quality meters LAQUA Series



Compact Spectroscopy Microscope



#### Diffraction Gratings



- VUV Synchrotron gratings  
- G400 coated master gratings  
- Custom gratings for astronomy and space flight



**Types of gratings:** Plane gratings, convex, concave, blazed / holographic or ruled gratings / Blazed with aberrations correction / OEM spectrometer or monochromator gratings / EUV to X-ray / Standard or custom capabilities

#### Synsco/Synphos Series CCD-Infrared InGaAs Detector



This is an optical spectrum detector used for a spectrometer



• For wide spectral acquisition

#### CRVS Series Small-size Spectrographs



Local compact spectrographs for small, portable equipment. Perfect for limited space and available for OEM supply.



#### Hyperspectral Imaging and Multichannel Spectrographs Hyperspectral Cameras



Miniature spectrometers optimized for CCD, CMOS and InGaAs linear array sensors to operate from UV through NIR range.



Model: IHR-0057C

Explore the future

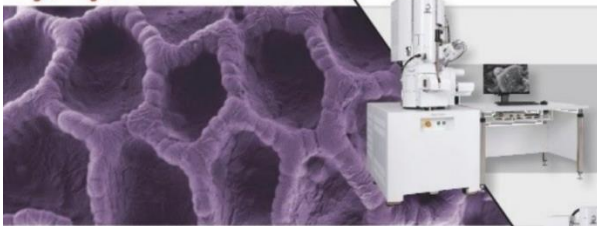
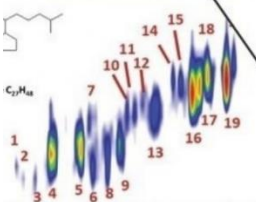
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Explore the future

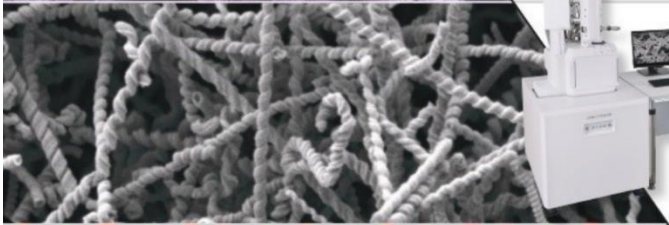
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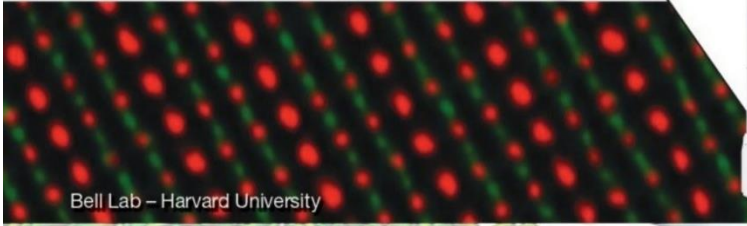
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## STEP INTO THE WORLD OF JEOL



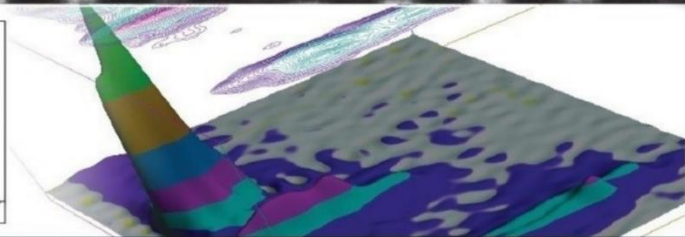
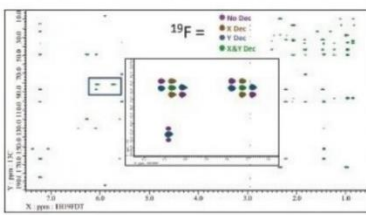
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- TEM
- SAMPLE PREP
- NMR
- MASS SPEC
- EPMA
- LITHOGRAPHY



Bell Lab – Harvard University



Osaka University



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**Quantum Design**  
INDIA




**Quantum Design: MPMS 3 Squid Magnetometer**  
 Temperature Range: 1.8K - 400K  
 Magnetic Field:  $\pm 7T$




**Quantum Design: PPMS DynaCool (Cryogen Free)**  
 Temperature Range: 1.8K - 400K  
 Magnetic Field:  $\pm 14T$




**Quantum Design: PPMS VersaLab (Cryogen Free)**  
 Temperature Range: 50K - 400K  
 Magnetic Field:  $\pm 3T$



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 (0.4 & 1  $\mu$  resolution)  
 Up to 180mm<sup>2</sup>/minute (resolution dependent)  
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 FastHall measurement in PPMS



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 Turn-key Broadband FMR spectrometer  
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 Email: info@qd-india.com





**ANALYTICAL  
SOLUTIONS  
GEARED FOR THE FUTURE**

**INORGANIC**

Atomic Absorption Spectrometer | ICP-OES | ICP-MS | Sample Digestion System



**CHROMATOGRAPHY**

Gas Chromatography | Headspace Technology | Customized GC Analyzers | Liquid Chromatography



**MOLECULAR SPECTROSCOPY**

UV-Vis, UV-Vis-NIR | FTIR, FTNIR | Fluorescence Spectrometers



**Organized by Team M2S**



**INNOVATIONS  
ENGINEERED  
FOR WORTHIER  
ANALYTICAL SOLUTIONS**

**THERMAL ANALYSIS**

TGA | STA (DTA)



TGA



DSC & STA

**HYPHENATED TECHNIQUES**

LC-ICPMS | TGA-IR | TGA-MS | TGA-GC/MS | TGA-IR-GCMS



TGA-IR-GCMS



TGA-MS



TGA-GC/MS



TGA-IR

**MASS SPECTROMETRY**

GCMS | LC/MS/MS | HPLC-ICP-MS Speciation



GC 2400™ with MS 2400™  
SQ Detector System



Clarus® SQ8 GCMS



QSight™ LC-MS/MS



HPLC-ICP-MS Speciation

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## ProLab Series Glove Box



ProLab series Glove box designed specifically for production and research applications. ProLab Glove Boxes are used in controlled atmospheres (dry boxes) or for use with hazardous materials. Protector Controlled Atmosphere Glove Boxes provide a leak-tight environment for work with contamination-sensitive materials.



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# Programme Booklet



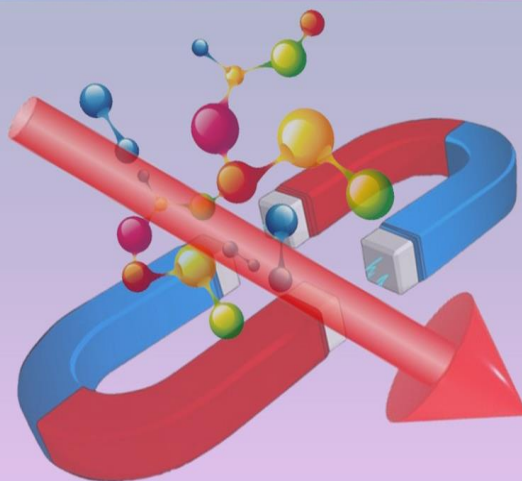
Modern Trends in Molecular  
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**5<sup>th</sup> – 8<sup>th</sup> November 2024**



Venue: AVR, RBM, AG-04  
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## Conveners

**Prof. Abhishek Mondal**  
**Prof. S. Ramasesha**

## Local Organizing Committee

**Dr. Awadhesh Narayan, Dr. Bhagwati Prasad,**  
**Dr. Soumen Ghosh, Dr. Susanta Hazra,**  
**Dr. Sujit Das, Dr. Veerabhadrrao Kaliginedi**



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