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BOOK OF ABSTRACTS

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Thursday, October 23rd		
12:15-13:00	***Welcome (soft drinks.)***	***Room 102 Tour 44-45***
13:00–13:10	***Introduction***	***Room 108 Tour 44-45***
Chair: Lorenzo Sorace		
13:15-13:45	**PL-1: Diana Serrano** ***Title: The Quantum Nature of Lanthanides: From Fundamentals to Applications***	
Chair: Grace Morgan		***Room 109 Tour 44-54***
14:00-14:25	**INV-1: Eugenio Coronado** ***Title: Spin-crossover materials for molecular electronics***	
14:30-14:55	**INV-2: Yann Garcia** ***Title: Developing tetranuclear Fe(II) spin crossover cages for gas sensing***	
15:00-15:30	***Coffee Break***	***Room 102 Tour 44-45***
Chair: Yann Garcia		***Room 109 Tour 44-54***
15:30–15:55	**INV-3: Rodrigue Lescouëzec** ***Title: Experimental approaches for probing the origin of cooperativity in a family of Fe_2Co_2 charge transfer complexes***	
16:00–16:25	**INV-4: Masamichi Nishino** ***Title: Stepwise Spin Transitions Studied by Elastic Interaction Models for Spin-Crossover Materials***	
16:30–16:55	**INV-5: Eliseo Ruiz** ***Title: Magnetism and Transport of Single-Molecule Spin-Crossover Systems***	
Friday, October 24th		
Chair: in progress		***Room 108 Tour 44-45***
9:00 - 9:30	**PL-2: Oscar CESPEDES** ***Title: Tuning the spin physics of metallic thin films via molecular interfaces***	
Chair: Eugenio Coronado		***Room 109 Tour 44-54***
9:45 - 10:10	**INV-6: Daniel R. Talham** ***Title: Interface and Matrix Effects on Spin Transition Solids***	
10:15 - 10:40	**INV-7: Osamu Sato** ***Title: Electric Polarization Switching between Symmetry Inequivalent Polar States Using Electron Transfer***	
10:45 - 11:15	***Coffee Break***	***Room 102 Tour 44-45***

***Chair:* Eva Rentschler**		***Room 109 Tour 44-54***
11:15 - 11:40	**INV-8:** Claude Piguet ***Title:* Luminescent Lanthanide Reading of Iron Spin Crossover: A Tale of Thwarted Love**	
11:45 - 12:10	**Inv-9:** Franc Meyer ***Title:* Dynamics and Cooperativity of Electron Transfer Induced Spin Transitions in Molecular Fe/Co Prussian Blue Analogues**	
12:15 – 13:40	***Lunch***	***Room 102 Tour 44-45***
13:40-13h45	***Presentation of the Olivier Kahn price by Michel Verdaguer***	***Room 108 Tour 44-45***
***Chair:* Daniel R. Talham**		
13:45 – 14:15	**PL-3:** Shin-ichi Ohkoshi ***Title:* Cyano-bridged metal complexes as platforms for multifunctional materials**	
14:30-14:55	**INV-10:** Aurelian Rotaru ***Title:* Dielectric Relaxation and Spin-State-Dependent Charge Transport in P(VDF-TrFE)/Spin-Crossover Nanofiber Composites**	
15:0 0-15:25	**INV-11:** Grace Morgan ***Title: in progress***	
15:30-16:00	***Coffee Break***	***Room 102 Tour 44-45***
***Chair:* Eliseo Ruiz**		***Room 108 Tour 44-45***
16:00–16:25	**INV-12:** Asuka Namai ***Title:* High-frequency magnetization dynamics in ε-iron oxide**	
16:30–16:55	**INV-13:** Ahmed Slimani ***Title:* Simulation Study of Spin-Crossover Coatings under Day–Night Cycles**	

Plenary lecture: Diana Serrano

Title. The Quantum Nature of Lanthanides: From Fundamentals to Applications

19th International Conference on Molecular Magnetism 2025
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Spin-crossover materials for molecular electronics

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Abstract

Electronic devices based on the spin-crossover phenomenon is strongly limited by the insulating character of the SCO complexes [1]. This limits the stability of the devices since high voltages and currents are needed to be applied to have an output signal. A possible solution to overcome this problem exploits the possibility of putting a thin layer of the SCO system in direct contact with a layer of graphene or other 2D semiconducting materials. In this case, we take advantage of the changes induced by the spin transition on the electrical or optical properties of the 2D material. In these hybrid devices the electrical current does not pass through the SCO but through the layer underneath, thus allowing to improve the endurance, performance, and detection of the spin state [2, 3].

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Developing tetranuclear Fe(II) spin crossover cages for gas sensing

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Abstract

The occurrence of spin crossover (SCO) usually induces different outputs, one of which is the colour change, an essential parameter for the design of a colorimetric sensor. Tetrahedral Fe^{II}-based metal organic cages have gained increasing attention as versatile SCO systems, owing to their unique ability to combine magnetic bistability with host–guest chemistry. Recent advances in ligand design and self-assembly strategies have enabled the construction of both face-capped $Fe^{II}_4L_4$ and edge-bridged $Fe^{II}_4L_6$ architectures, which display diverse SCO behaviors under thermal, chemical, or photonic stimuli. These cages serve as valuable models for understanding how factors such as ligand field strength, intermolecular interactions and guest encapsulation influence spin-state switching and distribution. Through a combination of magnetic susceptibility, ^{57}Fe Mössbauer spectroscopy, and crystallographic analysis, structure–function relationships have been systematically established. These studies demonstrate the potential of Fe(ii) SCO cages not only for probing fundamental structure–property relationships, but also for developing functional materials that integrate magnetic, optical, and host-guest responsiveness in the solid state.[1-4]

Herein, by symmetric modification of the ligand architecture, two complexes: a $Fe^{II}(L_1)_2$ mononuclear high-spin (HS) complex (**1**) and a $Fe^{II}_4(L_2)_6$ tetranuclear spin crossover cage (**2**) were constructed as colorimetric $NH_{3(g)}$ sensors, operating in the solid state. The sensing process is accompanied by a remarkable colour change from reddish brown (**1**) or light purple (**2**) to dark grey at room temperature. The cage presents a shorter response time (90 s) to $NH_{3(g)}$ compared to the complex (8 min) due to its empty cage structure, as revealed by single crystals X-ray diffraction, as well as by the large specific surface area increasing the adsorption rate of $NH_{3(g)}$. ^{57}Fe Mössbauer spectroscopy was employed to investigate the sensing mechanism around the metal centre. A conversion of 33% Fe^{II} ions to the low-spin (LS) state was observed in **1**@NH_3, after the substitution of $NH_{3(g)}$ molecules, leading to FeN_6 sites. The sensing mechanism of **2** also involves a HS to LS transition of Fe^{II} ions induced with a new FeN_6 centre, but non-coordinated BF_4^- anions were also found to react with NH_4^+ to form NH_4BF_4. These findings provide a solid foundation for exploring Fe^{II}-based coordination complexes as potential NH_3 gas sensors towards high nuclearity as well as tuneable porosity.[5]

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Experimental approaches for probing the origin of cooperativity in a family of Fe_2Co_2 charge transfer complexes

Rodrigue Lescouëzec [1], Yanling Li [1], Buqin Xu [1], Sadyia Sadyia [1], Geoffrey Gontard [1], Lise-Marie Chamoreau [1], Kevin Béneut [2], Paraskevas Parisiades [2], Benoit Baptiste [2], Maxime Deutsch [3], Damian Paliwoda [4], Shiteng Mi [4], Gabor Molnar [4], Nour-El-Islam Belmouri [5], Longhe Li [5], Mouhamadou Sy [4], Kamal Boukheddaden [5]

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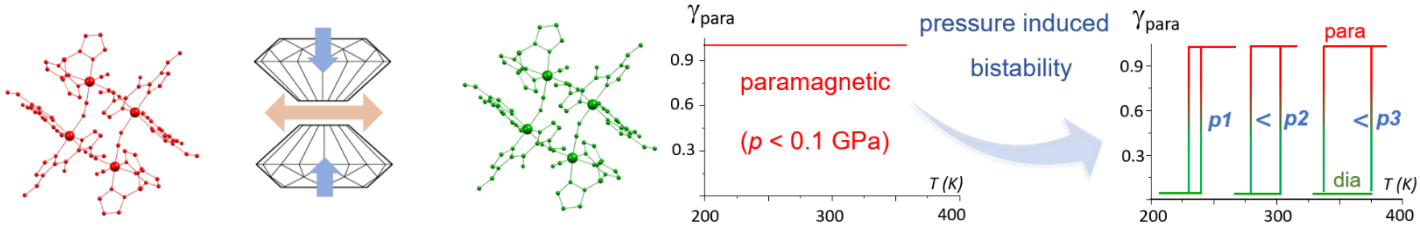
Cyanide-bridged FeCo charge transfer complexes that show controlable metal-metal electron transfer under temperature, pressure change or light irradiation are particularly attractive molecular switches. In these systems, the $Fe^{II}_{LS}Co^{III}_{LS} \Leftrightarrow Fe^{III}_{LS}Co^{II}_{HS}$ electronic state conversion is associated to drastic changes in optical, mechanical or magnetic properties. In the last years, we have been particularly interested in the study of family of Fe_2Co_2 square complexes show appealing behaviours under pressure application. In particular, in the complex $\{[Fe(Tp)(CN)_3]_2[Co(vbik)_2]_2\}(BF_4)_2$, we observed the emergence of a thermal bistability domain upon applying hydrostatic pressure (Scheme 1).[1] A combined study using Raman spectroscopy, magnetometry, and variable-pressure single-crystal X-ray diffraction enabled us to rationalize this phenomenon within the framework of a continuum mechanics model.[2] More importantly, this analysis allowed us to quantify the relative efficiency of distinct intermolecular pathways in transmitting the elastic interactions responsible for the hysteresis opening. In contrast with our first assumption based on simple structural description, the interactions involving the counter ions play a major role (rather than other supramolecular interactions). Further investigations based on optical microscopy and variable-pressure crystallography on related square complexes independently support this observation.[3,4] Overall, these experimental findings challenge the conventional empirical descriptions of cooperative effects in MMET systems. They highlight the need for systematic experimental investigations combined with advanced theoretical modeling to achieve a deeper understanding of the microscopic origin of cooperativity in these multistable materials.



Scheme 1. Pressure application on a Fe_2Co_2 paramagnetic complex lead to a thermal hysteresis opening that increases upon pressure increase.

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Stepwise Spin Transitions Studied by Elastic Interaction Models for Spin-Crossover Materials

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Abstract

Spin-crossover (SCO) materials show colorful ordered structures and switching phenomena induced by temperature change, pressure variation, light irradiation, etc. The elastic interaction arising from lattice distortion due to molecular size difference between the low-spin and high-spin molecules plays a crucial role in the cooperativity of those transitions. Frustration arising from a competiton between short-range and effective long-range interactions of elastic origin results in a variety of thermodynamic and metastable phases [1-7]. In this presentation we introduce our study of elastic interaction models for SCO materials. Through phase diagram analysis, we identified diverse patterns of thermally induced spin transitions with stepwise behavior [4–7]. The phase diagrams of the elastic interaction models often exhibit unusual features (Fig. 1, left), and stepwise transitions (Fig. 1, middle and right) reflect these characteristics. We demonstrate the properties of the phases arising from the competing interactions and discuss the mechanism of the stepwise transitions.

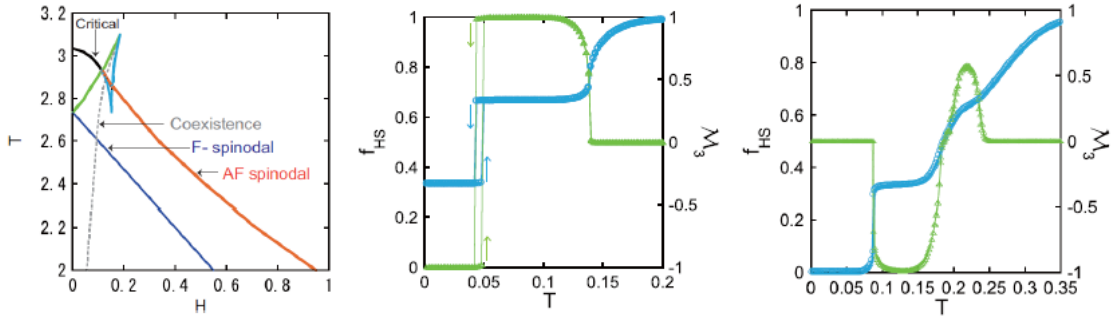

Fig. 1. (Left) Phase diagram for a model competing antiferromagnetic short-range and ferromagnetic long-range interactions, (middle) two-step spin transition , (right) four-step spin transition

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Magnetism and Transport of Single-Molecule Spin-Crossover Systems

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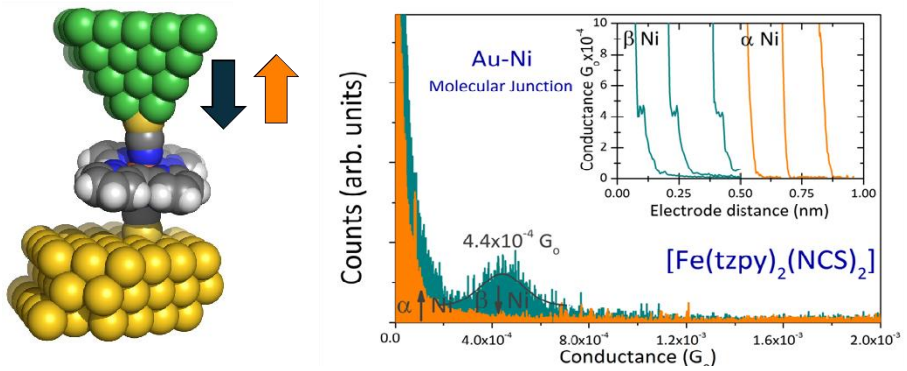
Abstract

Spin-crossover materials are challenging and surprising systems from both experimental and theoretical perspectives. In this presentation, I will discuss the findings of a spin-crossover system where a single molecule shows hysteresis behavior.[1] This phenomenon was unexpected, as hysteresis is typically associated with intermolecular cooperative interactions. In this case, the blocking of one of the molecule' s spin states hinders the spin transition, leading to hysteresis. Additionally, I will present results about the measurement of transport properties through a single molecule using a scanning tunneling microscope (STM). Some magnetic systems show magnetoresistance effects in single-molecule junctions. We were the first to report such behavior at room temperature.[2]

Figure : STM measurements of single-molecule transport



From a theoretical point of view, spin-crossover systems are a fundamental challenge, since initially very accurate post-Hartree Fock methods lead to worse results than those obtained with DFT methods. An additional challenge is to move from studying isolated molecules to periodic systems, which limits the methods to DFT or tight-binding methods. Results are presented on how to address this problem and methods that enable the fast screening of thousands of systems using both single-molecule calculations and the unit cell of the periodic system.[3]

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Plenary lecture : Oscar CESPEDES

Title. Tuning the spin physics of metallic thin films via molecular interfaces

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Interface and Matrix Effects on Spin Transition Solids

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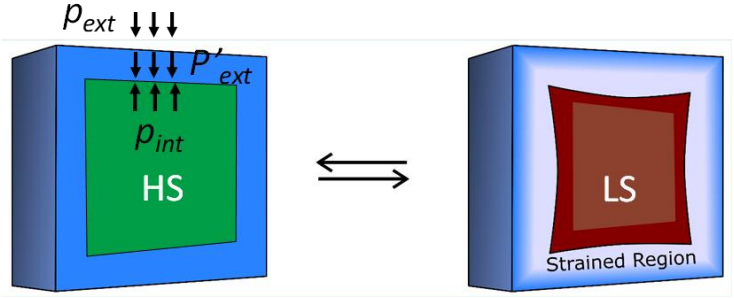
Abstract

If switchable spin-transition magnetic networks are to be incorporated into complex architectures for applications ranging from spintronics to mechanical actuators, how 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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Electric Polarization Switching between Symmetry Inequivalent Polar States Using Electron Transfer

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Abstract

The design and synthesis of novel molecular compounds, whose physical properties can be controlled by external stimuli, have attracted considerable attention. One of the most important of these properties is electric polarization. Many ferroelectric compounds have been developed, the polarization of which can be controlled by an electric field. However, achieving perfect polarization alignment by external stimuli other than an electric field is challenging due to the formation of a domain structure with a different polarization direction, which is caused by the presence of two or more symmetry-equivalent polar states. Recently, we proposed a strategy for achieving polarization switching via electron transfer in molecular crystals.[1] This strategy consists of two parts: synthesizing molecules that exhibit switching of their dipole moment via intramolecular electron transfer, and controlling their orientation to ensure that electron transfer occurs in the same direction. As the polarization switching occurs between symmetry-inequivalent, nondegenerate polar states with distinct physical properties such as entropy, magnetization, volume and absorption, the polarization can be switched with perfect polarization alignment by various external stimuli, including temperature, magnetic fields, pressure and light. The directional electron transfer induced by external stimuli results in a significant change in polarization, comparable to that observed in conventional ferroelectrics. Furthermore, the precise molecular design can be exploited to endow the polarization-switchable compounds with superior functionality. We will report on the polarization properties of several compounds, including heterometallic dinuclear [CoM] complexes (M = Cr, Fe and Ga), synthesized using our strategy.[1-4] These complexes exhibit a change in polarization via electron transfer in response to temperature, light and magnetic fields.

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Luminescent Lanthanide Reading of Iron Spin Crossover: A Tale of Thwarted Love

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Abstract

The concept of spin transition goes back to Pauling's description of the nature of chemical bonding and finds a satisfactory description within the ligand-field theory. The $3d^6$ open-shell metallic centers, as Fe(II), appear to be the most promising candidates for working as molecular-based magnetic and optical switches responding to thermal, pressure. electric or light-induced stimuli. The target energy balance between the ligand-field splitting Δ_{oct} and the electron pairing energy $P = 2B+4C$, which is crucial for inducing a usable spin crossover (SCO) process, can be tuned by the geometry and the nature of the coordination sphere around Fe(II). Distorted octahedral $[FeN_6]$ units, where N are heterocyclic nitrogen donors are recognized keys for this purpose, and non-symmetrical bidentate ligands, made of alternated heterocycles involved in five-membered chelates rings corresponds to some grail for inducing accessible SCO in $[Fe(N^{\frown}N')_3]$ chromophores.

The detection (i.e. reading) of the spin-state switching process at the molecular level appears as important as its implementation if profitable and socially acceptable applications such as sensor or as Q-bit are to be proposed. The best (*i,e.* easy access, highly selective and cheap) solution relies on the indirect SCO modulation of a long-lived luminescent signal observed in the visible part of the electromagnetic spectrum and originating from an appended earth-abundant trivalent lanthanide metal, a strategy proposed more than two decades ago, successfully realized once in a doped solid material,[1] and implemented only recently in isolated (supra)molecules (Figure).[2]

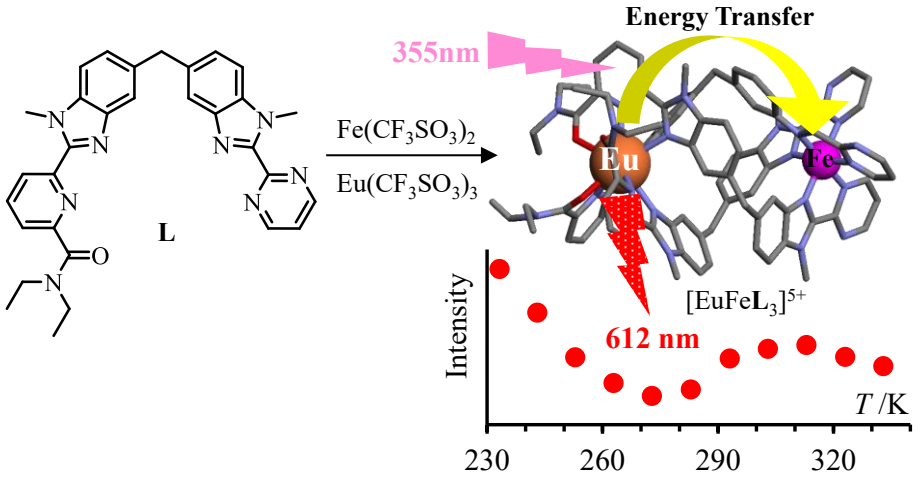

Figure : Molecular structure and light modulation of the spin crossover $[FeEu\mathbf{L}_3]^{5+}$ complex.

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Dynamics and Cooperativity of Electron Transfer Induced Spin Transitions in Molecular Fe/Co Prussian Blue Analogues

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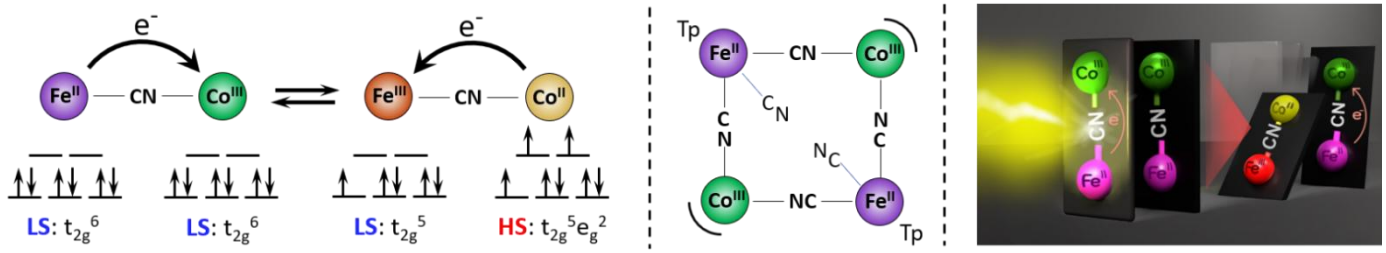
Abstract

Multimetallic systems offer new perspectives for light harvesting and energy storage in excited electronic and spin states. In this context we have investigated how elastic coupling between the individual metal sites in pyrazolate-based tri- and tetrairon(II) [2×2] grid complexes[1] or in some square Fe_2Co_2 Prussian Blue Analogues (PBAs)[2] influences the lifetimes of the excited charge transfer (CT) and spin states. Using a suite of time-resolved spectroscopic and X-ray diffraction techniques enabled to reveal correlations of spin and charge dynamics and of the structural evolution accompanying light excitation of the oligometallic systems.[3-7]

The focus of this presentation is on the elementary photophysical processes during electron transfer coupled spin transitions (ETCST) in selected FeCo or Fe_2Co_2 molecular PBAs with the aim of controlling and extending the lifetimes of excited states. To that end, time-resolved mid-IR and UV/vis pump-probe spectroscopies have revealed correlations of spin and charge dynamics of the photodriven ETCST in the oligometallic systems in solution.[5-7] This allowed, among other things, the first demonstration of a single-photon-induced cooperative ETCST at the molecular level, caused by elastic coupling of the {FeCo} subunits in a square Fe_2Co_2 PBA.[6]

Figure : ETCST process in FeCo PBAs[2] and illustration of the cooperative light-induced switching in a square Fe_2Co_2 PBA[6]



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Presentation of the Olivier Kahn price by Michel Verdaguer

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Cyano-bridged metal complexes as platforms for multifunctional materials

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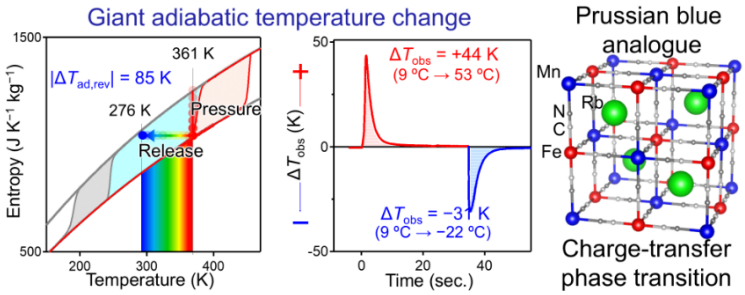
Abstract

Molecule-based materials offer a versatile platform for designing systems with diverse physical properties. Among them, cyano-bridged metal complexes have emerged as key candidates for multifunctional applications. Our work has demonstrated that these compounds can exhibit photo-switchable ferro- and ferrimagnetism, humidity-responsive magnetism, magnetization-induced second harmonic generation, proton conductivity, and multiferroic behavior.[1-3,6] In this presentation, we will introduce our recent research on functional cyano-bridged metal complexes.

Barocaloric material based on a charge-transfer phase transition: We synthesized a rubidium cyano-bridged manganese–iron–cobalt complex, $RbMn\{[Fe(CN)_6]_{0.92}[Co(CN)_6]_{0.08}\}\cdot 0.3H_2O$, exhibiting a pressure-sensitive charge-transfer phase transition. This transition, accompanied by thermal hysteresis, can be reversibly triggered by hydrostatic pressure, yielding a substantial barocaloric effect. Adiabatic temperature changes reach 74 K at 340 MPa and 85 K at 560 MPa. Direct measurements revealed shifts of +44 K during pressurization and −31 K during depressurization, with performance maintained over 100 cycles.[4] To probe ultrafast switching dynamics, we studied $Rb_{0.94}Mn_{0.94}Co_{0.06}[Fe(CN)_6]_{0.98}$, which undergoes a photoinduced phase transition near room temperature with a wide thermal hysteresis of 75 K.

Ultrafast photoswitching dynamics captured using streaming crystallography: Using a novel powder streaming technique combined with ultrafast X-ray diffraction, we captured transient structural changes on a sub-nanosecond timescale. The results indicate that photoinduced polarons initiate lattice expansion, and upon reaching a critical fluence, the full transition to the high-temperature phase completes within 100 picoseconds. These findings align with predictions from Landau theory and open new avenues for the dynamic control of material properties.[5]

Photoinduced charge-transfer-induced spin transition (CTIST) observed by ultrafast spectroscopy: We studied the photoinduced CTIST in 2D cyano-bridged Co–W assemblies. Ultrafast spectroscopy revealed a dynamic process of Co^{III}_{LS}-W^{IV} (LT) → Co^{II}_{LS}-W^{V} (transient photoexcited state) → CoIIHS-WV (HT), providing insights into the ultrafast CTIST mechanism.[6]



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Dielectric Relaxation and Spin-State-Dependent Charge Transport in P(VDF-TrFE)/Spin-Crossover Nanofiber Composites

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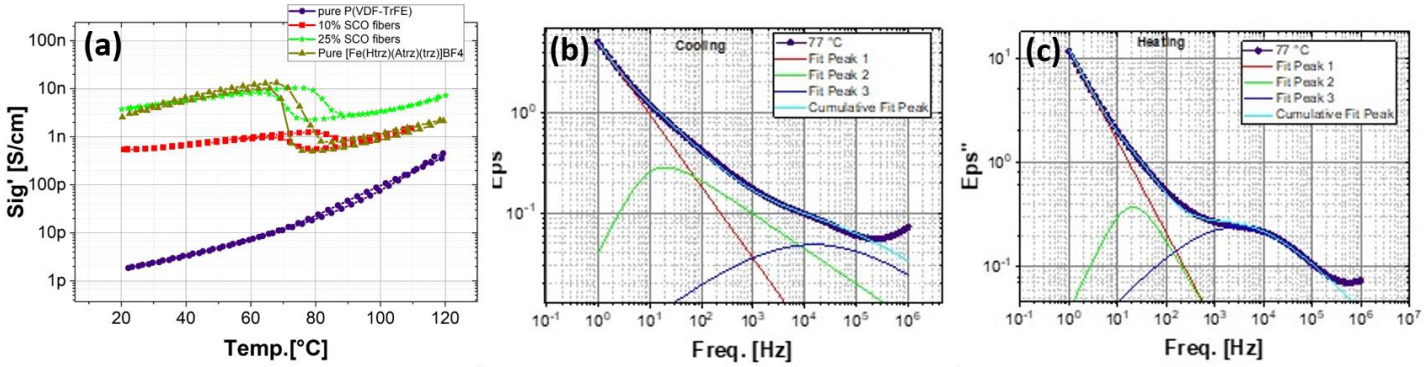
Abstract

This study explores the dielectric and charge transport properties of nanofiber composites combining the spin-crossover (SCO) complex $[Fe(Htrz)(Atrz)(trz)]BF_4$ with the ferroelectric copolymer P(VDF-TrFE). The materials were prepared as electrospun nanofibers containing 10 wt.% and 25 wt.% of the SCO complex, as well as blade-cast films with comparable composition. Broadband impedance spectroscopy measurements were conducted using a Novocontrol CONCEPT 40 dielectric spectrometer over the 0.1–10^6 Hz frequency range and between 20 and 120 °C. The analysis revealed that all systems exhibit thermally activated charge transport characteristic of hopping conduction. The inclusion of the SCO complex increases the overall conductivity while maintaining the materials in an insulating regime.

The dielectric spectra were analyzed using the Havriliak–Negami (HN) model, which allowed deconvolution of multiple relaxation processes arising from electrode polarization, dipole reorientation, and charge transport [1,2]. Comparison of the dielectric spectra in the low-spin (LS) and high-spin (HS) states showed a substantial reduction of the dielectric relaxation strength by nearly two orders of magnitude in the HS state. This behavior parallels the conductivity switching observed during the spin transition, confirming the strong coupling between electronic and spin degrees of freedom.

Figure 1: (a) Temperature dependence of the AC conductivity recorded on electrospun fibers of pure PVD-TrFE, 10% SCO, 25% SCO and $[Fe(Htrz)(Atrz)(trz)]BF_4$ complex respectively. Deconvolution of ε'' spectra recorded at 77 °C in (b) HS and (c) LS states.



Interestingly, the dielectric relaxation times in the composite nanofibers are one order of magnitude lower than in the pure SCO material, indicating that the polymer matrix modifies the charge carrier dynamics, likely by facilitating carrier hopping frequencies. These results demonstrate that embedding SCO complexes into a ferroelectric polymer matrix provides an effective way to engineer materials with tunable dielectric and charge transport properties, paving the way for multifunctional hybrid systems for sensing, memory, and spintronic applications.

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Grace Morgan

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High-frequency magnetization dynamics in ε-iron oxide

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Abstract

Magnetic moments in insulating magnetic materials can interact with AC magnetic field through several mechanisms. Among them, natural resonance—the zero-field ferromagnetic resonance originating from the gyromagnetic precession of magnetization—appears at the highest frequency. We have been investigating the natural resonance of ε-iron oxide (ε-Fe_2O_3), which exhibits one of the highest resonance frequencies among magnetic materials in the millimeter-wave region due to its large magnetic anisotropy. In addtion, owing to this anisotropy, the magnetization of ε-Fe_2O_3 responds to radio frequency (RF) magnetic field via Brownian rotation of the particles. In this presentation, we report our recent studies on the functionalities induced by such high-frequency magnetic dynamics, particularly in gallium-substituted ε-iron oxide (ε-$Ga_xFe_{2-x}O_3$).

Development of thin absorber utilizing impedance matching: In addition to the intrinsic millimeter-wave absorption of ε-$Ga_xFe_{2-x}O_3$ arising from natural resonance, the performance can be enhanced by satisfying the impedance-matching condition. We prepared a composite material consisting of ε-$Ga_xFe_{2-x}O_3$, a conductive component, and a resin matrix. The composite exhibits a complex permittivity ($\varepsilon = \varepsilon' - i\varepsilon''$) of $\varepsilon' = 19.4$ and $\varepsilon'' = 3.3$, and a complex permeability ($\mu = \mu' - i\mu''$) of $\mu' = 0.87$ and $\mu'' = 0.13$ at 79 GHz. By tuning the thickness to achieve impedance matching, we fabricated an ultrathin millimeter-wave absorber showing a reflection loss of −21.4 dB (99.3% absorption) at 79 GHz with a thickness of 213 ± 8 μm.

Enhancement of millimeter wave absorption and rotation properties by particle size effect: The particle size effect on millimeter-wave absorption was examined for ε-$Ga_xFe_{2-x}O_3$ ($x = 0.44 \pm 0.01$). Nanoparticles with average sizes of 16.9 nm, 28.8 nm, and 41.4 nm were synthesized. Millimeter-wave absorption and Faraday rotation spectra were measured using terahertz time-domain spectroscopy. As the particle size increased, the absorption magnitude rose from 4.6 dB to 9.4 dB, while the Faraday rotation angle increased from 9.1° to 18.4°, and the ellipticity from 0.27 to 0.52. These enhancements are attributed to changes in the ratio between surface and core regions of the nanoparticles.

Magnetic-field-induced frequency shift: We further investigated the effect of external magnetic fields on the natural resonance of ε-$Ga_xFe_{2-x}O_3$ nanomagnets. When the external field (H_{ex}) was switched between +3.5 kOe and −3.5 kOe, the resonance frequency shifted, for example, from 70 GHz to 81 GHz for $x = 0.46$. This field-tunable resonance enables a millimeter-wave switching functionality.

Heat dissipation through Brownian motion: ε-Fe_2O_3 nanoparticles exhibit the heating power of 80 W g^{-1} under RF magnetic field, attributed to the magnetization rotation accompanied by physical particle rotation. The heat-dissipation efficiency increases upon Ga substitution, owing to the enhanced saturation magnetization.

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Simulation Study of Spin-Crossover Coatings under Day–Night Cycles

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Abstract

Spin-crossover coatings change color and state with temperature, so they could help manage solar heating of walls/windows. Under realistic day–night cycles, it's hard to judge how basic parameters (film thickness, transition temperature, and optical contrast) shape the outcome without a simple, transparent model. In this work, we analyse spin-crossover (SCO) coatings with a coupled spin–optical–thermal model combining mean-field spin kinetics, Beer–Lambert absorption, and heat diffusion through the SCO coating and wall. Under representative day/night cycles, we quantify how film thickness (ω) and ligand-field splitting (Δ) affect the evolution of n_{HS} during day–night cycling, optical attenuation at the SCO/wall interface, interior wall temperatures, and the characteristic time to reach a periodic regime (τ). Within the examined ranges, increasing ω lowers transmitted intensity, an intermediate ω minimises τ, and Δ sets the operating temperature window. We also assess a two-layer configuration, which further reduces wall temperature at the cost of a higher τ.

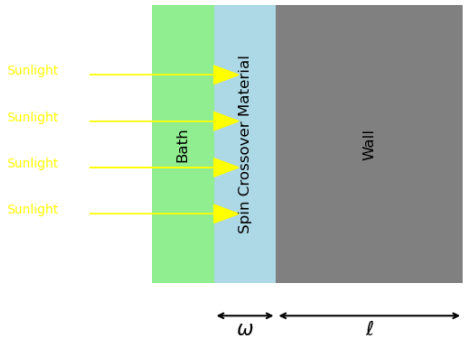

Figure: Geometry and boundary conditions used in the simulations. From left to right: ambient *bath* supplying time-dependent light $I_0(t)$ and temperature $T_B(t)$; SCO coating of thickness ω with spin-dependent absorption; wall of thickness ℓ.