

## Poster Timetable

**Monday 14<sup>th</sup> June 2021**

**Session 1.1**

19.30 – 19.55 (UK time, UTC+1)

[zoom.us/j/93870750691](https://zoom.us/j/93870750691)

Rm	Abs	Presenter	Title
1	316	Leonel Llanos Silva	Ab initio study of the quantum tunnelling of magnetization in bimetallic dysprosium single molecule magnets
2	79	Daniel Cutler	Small ligands with giant potential: Building large FeIII-O clusters from simple ligands
3	144	Carmen María Atzin Macedo	Synthesis and spectroscopic characterization of Ni(II), Co(II) and Mn(II) complexes derived from novel Schiff base
4	191	Brittany Grimm	High-Field EPR Study of the Spin-Crossover Transition in a Mn(III) Complex
5	185	Jason Yu	Computational Characterization of Molecular Spin Qubits using Density Functional Theory
6	85	Ashlyn Hale	Large Fe22 and Fe24 clusters: Synthesis, structure, and magnetic couplings via magnetostructural correlations and DFT
7	319	Daniel Lussier	The Structural, Electrochemical, and Magnetic Properties of Diuranium Complexes Containing an Organic, Redox-Active Bridge
<a href="https://zoom.us/j/97439940767">zoom.us/j/97439940767</a>			
8	80	Theocharis Stamatatos	Deposition studies of a new {Dy2} single-molecule magnet on graphene-like substrate
9	27	Mark Turnbull	Nearly isotropic AFM spin ladders: Structure and magnetism
10	301	Myron Huzan	Single-ion magnetism in the extended solid-state: insights from X-ray absorption and emission spectroscopy
11	43	Itziar Oyarzabal	A redox-active coordination chemistry approach to magnetic and/or conductive materials
12	148	Rosa Diego Creixenti	A mononuclear spin-crossover complex describing four distinct thermal routes
13	294	Mariana Velho	[Au(dspdt)2]: a conducting neutral bis(1,2-dithiolene) gold complex with a unique crystal structure
14	340	Andreas Kourtellaris	A microporous Co(II) - based 3-D metal organic framework built from magnetic infinite rod-shaped secondary building units
<a href="https://zoom.us/j/91766287448">zoom.us/j/91766287448</a>			
15	69	Anne Lüpke	Filling the gap in the metallocrown family: The 9-MC-3 chromium metallocrown
16	295	Jorge Navarro Giraldo	DFT study of Cobalt-based single-molecule magnet deposition on graphene
17	334	Krishnendu Kundu	Massive 9 GHz Hyperfine Clock Transition in a Lu(II) Molecular Spin Qubit
18	158	Aleksandra Pacanowska	Surface Deposition of CN-bridged Magnetic Sponges
19	14	Rubén Turo-Cortés	Reversible guest-induced gate-opening effect observed in spin crossover two-dimensional Hofmann Clathrates
20	115	Maria Sara Raju	Role of Vibronic coupling in the Magneto-Chiral Dichroism of Paramagnetic Complexes Exhibiting Helical Chirality

Monday 14<sup>th</sup> June 2021

Session 1.2

19.55 – 20.20 (UK time, UTC+1)

[zoom.us/j/93870750691](https://zoom.us/j/93870750691)

Rm	Abs	Presenter	Title
1	140	Walter Cañón-Mancisidor	Slow Magnetic Relaxation of a Hybrid Inorganic-Organic Ytterbium Complex
2	182	Daniel Aravena Ponce	Choosing between vibrational and Crystal field tuning for improvement of high-performance Single Molecule Magnets.
3	151	Lorena Martínez	Exchange coupling in a thiocyanato-bridged copper(II) chain: computational approach to magnetostructural correlations
4	193	Robert Stewart	Radical-lanthanide ferromagnetic interaction in a Dy(III) bis-phthalocyaninato complex
5	157	Michał Magott	The unexpected impact of humidity on the photoswitching of cyanide-bridged molecular magnets
6	204	Elly Daniels	Synthesis, structural analysis, and magnetic properties of molecular Bi-Mn-oxo and Pb-Mn-oxo coordination cages
7	307	Alexandre Vincent	Lanthanide-Cobalt bis-Dithiolene Compounds Exhibiting Significant Ferromagnetic Exchange and Single Molecule Magnetism
<a href="https://zoom.us/j/97439940767">zoom.us/j/97439940767</a>			
8	91	Vassilis Tangoulis	Spin Crossover Phenomenon and Nano-Topographic Study in Microcrystals and Nanoparticles of 2-D Hofmann-type polymers
9	291	Mario Pacheco	Magnetic properties of novel mononuclear Re(II) complexes with azole-type ligands
10	103	Céline Pichon	Trinuclear cyano-bridged [Cr <sub>2</sub> Fe] complexes: to be or not to be a good SMM, just a matter of straightness?
11	314	Brenna Cashman	Toward heavy pnictogen ligated single molecule magnets
12	78	Guillem Gabarró-Riera	Facile surface functionalization with luminescent and magnetic lanthanoid Schiff base complexes
13	192	Dandan Lou	Molecule-based metal-organic magnets with large coercivity and ordering temperatures up to 242°C
14	283	Thomas Morrison	Investigating origins and control of slow magnetic relaxation in Ni(III) octahedral complexes
<a href="https://zoom.us/j/91766287448">zoom.us/j/91766287448</a>			
15	186	Tom Bennett	A Ring of Rotaxanes
16	200	Vijay Singh Parmar	Probing relaxation dynamics in Dy-Aryloxide Single-Molecule Magnets
17	277	Jonatan Petersen	Magnetic interactions in lanthanide dimers: The role of the bridging ligand
18	188	Wojciech Sas	Nanotubes of Prussian blue and its Cr analog obtained by electrodeposition method
19	96	Aman Ullah	Theoretical insights into spin-electric couplings and vibronic relaxation pathways in clock-like molecular spin qubit: [Ho(W <sub>5</sub> O <sub>18</sub> ) <sub>2</sub> ] <sup>9-</sup>
20	278	Félix Houard	Water-dependent crystallization of infinite and finite Single-Chain Magnets

**Tuesday 15<sup>th</sup> June 2021****Session 2.1**

11.50 – 12.15 (UK time, UTC+1)

[zoom.us/j/93234805108](https://zoom.us/j/93234805108)

Rm	Abs	Presenter	Title
1	66	Reshma Jose	Decisive Role of Spin-States and Spin-Coupling in Dictating Selective O <sub>2</sub> Adsorption in Chromium(II) Metal-Organic Framework
2	81	David Harding	Symmetry-Breaking and Light Activation in Iron(III) Spin Crossover Complexes
3	173	Krishna Kaushik	Reversible Photo and Thermo-induced Spin-State Switching in a heterometallic {5d-3d} W <sub>2</sub> Fe <sub>2</sub> Molecular Square Complex
4	285	Kilian Jutglar	Twistable dipolar aryl rings as electric field actuated conformational molecular switches
5	133	Naoka Amamizu	Theoretical study on the difference in single-molecule electron conductivity of paddlewheel-type binuclear Cr(II) complexes between antiferromagnetic and ferromagnetic states
6	131	Irina Kühne	Investigation on ligand substituent effects on Mn(III) Spin Crossover Complexes
7	222	Ismael Francisco Diaz Ortega	In search of Co <sub>3</sub> <sup>II</sup> based zero field SMMs based on tripodal ligands
8	174	Katarzyna Rzepka	Lanthanide Single Molecule Magnets with azahelicenes
9	211	Guanping Li	Design of Thiocyanido-bridged FeII-HgII Frameworks Revealing Chirality, Spin-crossover and Photomagnetism
10	226	Andrea Albino	First-Principles Spin Dynamics Under Terahertz Irradiation
<a href="https://zoom.us/j/93990174843">zoom.us/j/93990174843</a>			
11	87	Lingyi Meng	A smart post-synthetic route towards [Fe <sub>2</sub> Co <sub>2</sub> ] molecular capsules with electron transfer behaviour
12	275	Cristian Enachescu	Multiscale out-of-equilibrium dynamics in spin-crossover molecular materials described by a three thermalisation scales model
13	156	Xiu-Fang Ma	Layered Lanthanide Phosphonates Ln(2-qpH)(SO <sub>4</sub> )(H <sub>2</sub> O) <sub>2</sub> (Ln = La, Ce, Pr, Nd, Sm, Eu): Structures, Magnetic and Luminescent Properties
14	127	Hagen Kämmerer	What dictates structural changes in a Mn-Ln SMM system using N-methyldiethanolamine?
15	142	Moya Hay	Ligand Tuning in Cobalt Complexes for Valence Tautomerism
16	164	Alejandro Gaita-Ariño	Qualitative insights on molecular design oriented towards spin dynamics: spin relaxation and spin excitation
17	286	Yoshiro Sekine	Controlled intra-lattice electron transfers in tetraoxolene-bridged two-dimensional layers by temperature and guest molecules
18	120	Jonathan Fowler	Supramolecular Assemblies of [n]-Rotaxanes as Potential Quantum Logic Gates
19	41	Selena Lockyer	Controlling the interactions and conformation of multi-qubit systems using hybrid rotaxanes
20	166	Mukesh Singh	Host-guest induced magnetic features in dia/paramagnetic coordination capsules.

**Tuesday 15<sup>th</sup> June 2021**

**Session 2.2**

**12.15 – 12.40 (UK time, UTC+1)**

[zoom.us/j/93234805108](https://zoom.us/j/93234805108)

Rm	Abs	Presenter	Title
1	63	Arup Sarkar	Modulating Magnetic Anisotropy in Ln(III) Single-Ion Magnets using an External Electric Field
2	179	Raúl Santiago Piera	Tuning magnetism and conductivity in 2D covalent organic radical frameworks via mechanical compression
3	207	Subrata Ghosh	ON/OFF Photo-Switching and Thermo-Induced Spin Crossover with Cooperative Luminescence in a 2D Iron(II) Coordination Polymer
4	259	Richard Collins	Lanthanide SMMs; it's Plane to See
5	107	Yasutaka Kitagawa	Quantum design of ferromagnetic homonuclear bimetallic complexes based on orbital counter-complementarity
6	181	Alessio Nicolini	Tetrairon(II) Extended Metal Atom Chains as Single-Molecule Magnets
7	90	Akito Fujisawa	Anomalous Phase Transition Observed in Nanosize Tetratitanium Heptoxide
8	221	Katarzyna Rogacz	Photochromic dithienylethenes for the construction of photoswitchable quantum nanomagnets
9	231	Kunal Kumar	Effect of lanthanides on magnetic exchange-coupling and second harmonic generation
10	311	Michael Baker	The electronic structure and single-ion magnetism of linearly coordinated Mn(I), Fe(I), Co(I), and Ni(I) doped within lithium nitride crystals quantified by X-ray spectroscopy

[zoom.us/j/93990174843](https://zoom.us/j/93990174843)

11	240	Xin-Hua Zhao	Multiple Transition Dynamics: Spin Transition Coupled with Structural Phase Transition
12	168	Simen Sopp	Exceptionally Clean Single-Electron Transistors from Solutions of Pleio-Soluble Molecular Graphene Nanoribbons
13	143	Xin-Yi Wang	Molecular Magnetic Materials Based On $[\text{Mo}^{\text{III}}(\text{CN})_7]^{4-}$ Unit
14	315	Masooma Ibrahim	Polyoxometalate-Based High-Spin Functional Clusters
15	28	Jett Tao Janetzki	Predicting Transition Temperature in Valence Tautomeric Molecular Switches: A Computational and Experimental Study
16	132	Pablo Sevilla	Growth of Lanthanide-based 2D MOFs on silicon surfaces
17	150	Mohammad Reza Safari	Towards single-molecule-scale studies of enantioselective adsorption of chiral molecules on ferromagnetic surfaces
18	31	Palmerina Gonzalez Izquierdo	Crystal and Magnetic structures and Dielectric phase transition of the novel Organic-Inorganic Hybrid Halometallate compound: (quinuclidinium)[FeCl <sub>4</sub> ]
19	209	Alessandro Soncini	Quantum spin toroidicity in molecular spin rings
20	197	Marco Coletta	Biscalix[4]arene-supported metal clusters

**Wednesday 16<sup>th</sup> June 2021****Session 3.1**

11.50 – 12.15 (UK time, UTC+1)

[zoom.us/j/93234805108](https://zoom.us/j/93234805108)

Rm	Abs	Presenter	Title
1	213	Rupesh Tiwari	Modelling Magnetic Molecule Based Molecular Spin Transistor
2	255	Kenta Imoto	A pentacyanonitrosylferrate-based magnetic one-dimensional metal assembly exhibiting photo-induced switching of second harmonic generation
3	50	Nikolaos Konstantinidis	Discontinuous quantum and classical magnetic response of the pentakis dodecahedron
4	98	Athanasios Mavromagoulos	Synthesis and characterisation of CuII-GdIII complexes.
5	106	Yoshio Teki	$\pi$ -Topology and Ultra-Fast Excited-State Dynamics of Remarkably Photo-stabilized Pentacene Derivative Utilizing Radical Substituents
6	261	Jana Dubnická Midlíková	Development of FTIR spectroscopy in high magnetic fields
7	205	Anatoly Melnikov	Multimodal THz waveguides at EPR endstation of Novosibirsk Free Electron Laser: construction and overall performance
8	46	Xinghui Qi	In-Depth Investigation of Photomagnetic Compounds Based on Octacyanidometallates
9	161	Giang Truong Nguyen	Computational investigation of the magnetization blocking mechanism in exchange-coupled lanthanide single-molecule magnets
10	239	Jonas Braun	Quenching of QTM in Lanthanide Complexes with Semiquinonate Radical Ligands
<a href="https://zoom.us/j/93990174843">zoom.us/j/93990174843</a>			
11	111	Yao Binling	A dual-capping tetrazine ligand in favour of both trigonal prismatic geometry and strong magnetic coupling
12	243	Alessandro Chiesa	Molecular spin qubits for quantum simulation of light-matter interactions
13	147	Abinsah Swain	{Ru2Dy2} Butterflies: Examples of 4d-4f Single Molecule Magnets
14	214	Maja Dunstan	Crystal field splitting and exchange interactions in a lanthanoid-semiquinonate complex
15	232	Dominik Czernia	Effect of proton irradiation on magnetic properties of two-dimensional Ni(II) molecular magnet
16	149	Javier Cepeda	MOFs based on cobalt and 2-aminoisonicotinate behaving as field-induced SMMs: developing magnetic sensors
17	169	Jack Neill	Ab initio study of metal-ligand interactions and their role in altering magnetic properties of linear homoleptic two-coordinate transition metal complexes.
18	196	Gabriela Handzlik	Lanthanide complexes with carbo[6]helicene o-quinones
19	269	Emily Payne	Magnetic Exchange in Anderson-Type 3d Transition Metal Clusters
20	217	Diana Plesca	Unexpected Light-Induced Thermal Hysteresis in Matrix Embedded Low Cooperative Spin Crossover Microparticles

**Wednesday 16<sup>th</sup> June 2021****Session 3.2**

12.15 – 12.40 (UK time, UTC+1)

[zoom.us/j/93234805108](https://zoom.us/j/93234805108)

Rm	Abs	Presenter	Title
1	109	Sourav Dey	An In Silico Study of Gd <sub>2</sub> @C <sub>2n</sub> (15 ≤ n ≤ 40) EMFs: Estimation of Record High Magnetic Exchange and Magnetic Anisotropy
2	262	Yue Xin	Luminescent Cyanido-bridged DyIII-CoIII Framework Showing Solvent-driven Switchable Single-molecule Magnet Behavior
3	82	Xin-Da Huang	Reversible Cycloaddition Reactions of Dysprosium-Anthracene Compound Following Luminescent and Magnetic Switching
4	244	Daniel Martins	Hyperfine Spectroscopy of Cr7Ni Heterometallic Qubits
5	210	Rie Suizu	Clarification of the origin of the frustration-induced phase transition in reduced diamond lattice
6	18	Mario Falsaperna	Exploring the magnetocaloric effect in the Ln(HCO <sub>2</sub> )(C <sub>2</sub> O <sub>4</sub> ) family of Metal-Organic Frameworks
7	279	Asmita Sen	A Computational Assessment on a Series of High-Valent Fe/Mn-oxo/hydroxo Complexes, Revealing the Impact of Inner Electronic Structure on Their Reactivity
8	67	Georgios Velkos	Dy <sub>2</sub> O-Clusterfullerenes: Strong Magnetic Anisotropies and Fullerene-Dependent Single Molecule Magnetism
9	249	Olaf Stefanczyk	Photoswitchable high-dimensional octacyanidometallate-based networks
10	183	Simone Chicco	Controlled coherent dynamics of [VO(TPP)], a prototype molecular nuclear qudit with an electronic ancilla
<a href="https://zoom.us/j/93990174843">zoom.us/j/93990174843</a>			
11	92	Jing Li	Manipulation of Molecular Qubits by Isotope Effect on Spin Dynamics
12	300	Gemma Gransbury	Valence Tautomerism in Bis(dioxolene)-Bridged Dinuclear Cobalt Complexes: Correlating Two-Step Transitions with Redox and Mixed-Valence Properties
13	251	Magdalena Ceglarska	Magnetic investigations of monocrystalline [Co(NCS) <sub>2</sub> (L) <sub>2</sub> ] <sub>n</sub> : new insights into single-chain relaxations
14	224	Maria Brzozowska	High-performance tetrahedral ErIII SMMs.
15	159	Diana Visinescu	Cyanido-bridged {FeIII LnIII} heterobimetallic chains assembled through the [FeIII{HB(pz) <sub>3</sub> (CN) <sub>3</sub> }- complex as metalloligand: Synthesis, crystal structure and magnetic properties
16	171	Zhenxing Wang	Controlling Electron Spin Decoherence in Nd-based Complexes via Symmetry Selection
17	40	Kira Vostrikova	The lanthanide complexes of the tripodal nitroxyl radicals
18	152	Fabio Santanni	Synthesis of a Novel Set of Hydrogen-Free Complexes of 1,3,2-Dithiazole-4-thione-5-thiolate Ligand as Potential Spin Qubits
19	33	Emma Regincos Marti	Study on a family of Ln(III) highly coordinated complexes with a short axial Ln–F bond
20	170	Silvia Gimenez-Santamarina	Towards peptide-based magnetic multistate memristive materials