# MA 14: Focus Session: Frustrated Magnetism and Local Order (joint session MA/TT)

Recent experimental findings illustrate unexpected spin glass behavior in a variety of frustrated magnets. Often their description goes beyond conventional pictures of spin glasses. For instance, the interplay of antiferromagnetism and spin glass behavior was recently studied. Such systems could be used to study the gradual evolution of spin glass behavior in an itinerant magnet without a change of the crystallographic environment. In this context, the discovery of the so-called self-induced spin glass in elemental neodymium showed that glassy behavior can even exist in the absence of disorder, leading to local magnetic order in the absence of long-range order. This focus session brings together experts from different subfields of frustrated magnetism and with different experimental and theoretical expertise, in order to exchange conceptual ideas beyond "traditional" paradigms of spin glasses and frustrated magnetism. These conceptual ideas are linked to fields such as artificially built frustrated magnets (e.g. spin ice), multi-well systems with complex dynamics, or fragile magnetic systems that may exhibit complex magnetic order.

Coordinators: Daniel Wegner and Alexander A. Khajetoorians (Radboud University, Nijmegen)

Time: Tuesday 9:30–13:15 Location: H 1058

**Invited Talk** MA 14.1 Tue 9:30 H 1058

**Neutron scattering studies of spin-freezing phenomena at quantum phase transitions** — •Christian Pfleiderer — School of Natural Sciences, Department of Physics, Technical University of Munich, D-85748 Garching, Germany — Centre for QuantumEngineering (ZQE), Technical University of Munich, D-85748 Garching, Germany — Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, D-85748 Garching, Germany — Munich Centre for Quantum Science and Technology (MCQST), Technical University of Munich, D-85748 Garching, Germany

A cornerstone of the statistical and thermal physics of condensed matter systems concerns their energy landscape and the associated ergodicity. Conventional and topologically non-trivial forms of long-range magnetic order represent weak forms of non-ergodicity that allow to explore classical and quantum dynamics, as well as the origin and nature of topological protection. In contrast, strong forms of non- ergodicity related to glassy configurations and freezing transitions permit the comparison of quantum versus thermally driven relaxation as constrained, e.g., by disorder. Combining the results of neutron depolarization, neutron diffraction, and neutron spectroscopy with magnetization and ac susceptibility measurements, similarities and differences of spin freezing phenomena at selected quantum phase transitions will be presented. This includes the putative formation of reentrant spin glass behaviour in $Fe_{1-x}Cr_x$, a Kondo cluster glass in $CePd_{1-x}Rh_x$, and a spin liquid in $HgCr_2Se_2$ under pressure.

**Invited Talk** MA 14.2 Tue 10:00 H 1058

**Frustrations, glassiness and complexity of spin systems with large spatial dimension** — •Mikhail Katsnelson — Radboud University, Nijmegen, Netherlands

It was suggested some time ago [1] that spin system can behave as a glass without disorder, due to frustrations only (self-induced spin-glass state). Recent experimental discovery of glass-like magnetic state in elemental Nd at low temperatures [2] creates a very strong motivation to improve our theoretical understanding of such an opportunity. We have shown [3] that the glassiness without disorder can be derived quite rigorously for classical Heisenberg model in the limit of large spatial dimension, where an accurate and controllable mathematical treatment turns out to be possible.

For frustrated quantum spin systems, the sign structure of the ground state has a high complexity, in a sense that the machine learning of this structure is very difficult [4]. This problem however can be mapped to the classical Ising model of a very large dimension which allows to reach a progress in determining this sign structure [5].

[1]. A. Principi and M. I. Katsnelson, Phys. Rev. B 93, 054410 (2016); Phys. Rev. Lett. 117, 137201 (2016). [2] U. Kamber et al, Science 368, eaay6757 (2020); B. Verlhac et al, Nature Phys. 18, 905 (2022). [3] A. Mauri and M. I. Katsnelson, arXiv:2311.09124. [4] T. Westerhout et al, Nature Commun. 11, 1593 (2020). [5] T. Westerhout, M. I. Katsnelson, and A. A. Bagrov, Commun. Phys. 6, 275 (2023).

**Invited Talk** MA 14.3 Tue 10:30 H 1058

**Self-Induced Spin Glass Phase and Thermally Induced Order in dhcp Nd** — •Anders Bergman — Uppsala University, Uppsala, Sweden

Among the wide variety of magnetic orders found in frustrated magnets, one of the most intriguing phases is manifested by the spin glass state where the magnetization exhibit glassy dynamics, including ageing and memory effects. The peculiar dynamics of spin glass materials has historically been associated with disorder where magnetic frustration can cause an energy landscape with several local minima combined with larger energy barriers, resulting in non-ergodic behavior and glassy dynamics.

Recent theoretical and experimental findings have however indicated the existence of glassy dynamics in a material with limited chemical disorder: elemental and crystalline Nd [1]. In this talk, we will present results indicating that: I) the low temperature state of dhcp Nd can be described as a self-induced spin glass and II) dhcp Nd undergoes a phase transition from the self-induced spin glass phase to an ordered spin-spiral phase with increasing temperature [2].

Using first-principles DFT calculations of magnetic exchange interactions combined with atomistic spin dynamics simulations we can show that the complex magnetism of dhcp Nd is driven by an intrinsic frustration of the exchange interactions between Nd atoms at the cubic and the hexagonal sites in the dhcp structure.

[1] U. Kamber, et. al, Science 6757 368 (2020)
[2] B. Verlhac, et. al, Nature Physics 905 18 (2022)

MA 14.4 Tue 11:00 H 1058

**Spatially resolved aging and rejuvenation in a self-induced spin glass** — •Lorena Niggli[1], Julian H. Strik[1], Zhengyuan Liu[1], Anders Bergman[2], Mikhail I. Katsnelson[1], Daniel Wegner[1], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Spin glasses are a puzzling form of magnetic matter lacking long range order and possessing multiple relaxation time scales indicative of aging. These findings are based on ensemble thermodynamic measurements, which leave more to be known about the behaviour of the magnetization locally. Recently, we have discovered that the low temperature magnetic phase of elemental neodymium behaves like a proposed self-induced spin glass relying solely on spin frustration in the absence of disorder for glassiness [1,2]. Here, we explore the aging behaviour of Nd(0001) using spin-polarized scanning tunneling microscopy in varying magnetic fields. We observe a transition from an initial state, reached after cooling into the glass phase, towards a distinct final state, as we perturb the system. Temperature cycling allows us to rejuvenate the system back into its initial state, which hints towards a thermally written memory in this glassy system. Using a new analysis method, we quantify the favourability of the observed local order as well as investigate its link to the energy landscape.

[1] U. Kamber et al., Science 368 (2020).
[2] B. Verlhac et al., Nature Physics 18 (2022).

MA 14.5 Tue 11:15 H 1058

**Multipolar order in the 5$d$ double perovskite $Ba_2MgReO_6$ from DFT+DMFT** — Maximilian E. Merkel and •Claude Ederer — Materials Theory, ETH Zürich, Switzerland

We establish the effect of electronic correlations and strong-spin-orbit coupling on the emergence of the insulating state and the quadrupolar order in the magnetically frustrated 5d double perovskite $Ba_2MgReO_6$ (BMRO). BMRO exhibits a tetragonally distorted paramagnetic phase below $T_q \sim 33\,K$ and a non-collinear magnetically ordered state below $T_m \sim 18\,K$. Using density functional theory in combination with dynamical mean-field theory (DFT+DMFT), we demonstrate that BMRO should be classified as a normal Mott insulator where the spin-orbit coupling is not crucial for the formation of the insulating state. Our calculations further reveal a subtle interplay between the electronic quadrupolar order and the Jahn-Teller distortion, where the primary instability is of electronic origin but the coupling to the structural distortion determines the specific character of the emerging order.

**15 min. break**

**Invited Talk** MA 14.6 Tue 11:45 H 1058

**Frustrated Quantum Devices: Pathways to leverage exotic order in novel spintronic technologies** — •James Analytis — University of California at Berkeley, 366 Physics North, Berkeley, CA 94705, USA

Materials at the boundary of critical phase transitions are of significant fundamental interest, not least due because of their connection to unconventional superconductivity and quantum magnetism. One characteristic shared by many such systems is the presence of coupled order parameters that underlie these phase transitions. Here, we explore how this coupling manifests in the response of these materials when driven out of equilibrium by applied currents. We demonstrate how magnetic and charge textures can be electrically manipulated, suggesting possible applications for exotic materials in spintronics technologies.

MA 14.7 Tue 12:15 H 1058

**Noncoplanar and chiral spin states on the way towards Néel ordering in fullerenes** — •Attila Szabó[1], Sylvain Capponi[2], and Fabien Alet[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Laboratoire de Physique Théorique, Toulouse, France

Magnetic ordering can be detected in finite lattices through the emergence of Bragg peaks in ground-state structure factor or through the spectrum of low-energy excited states, which form an Anderson tower of states generated by Goldstone modes of the incipient symmetry breaking. In this talk, I will generalise these methods to large fullerenes, where incipient Néel ordering on the network of hexagonal faces is frustrated by a low density of pentagons. Using high-accuracy variational Monte Carlo based on group-convolutional neural networks, we obtain the symmetry-resolved low-energy spectrum of the spin-1/2 Heisenberg model on several highly symmetric fullerene geometries, including the famous $C_{60}$ buckminsterfullerene. We show that their correlation functions contain high-intensity Bragg peaks consistent with Néel-like ordering, while the low-energy spectrum is organised into a tower of states. Competition with frustration, however, turns the simple Néel order into a noncoplanar one. Remarkably, we find and predict chiral incipient ordering in a large number of fullerene structures. Our findings may have interesting ramifications for the nature of superconductivity in metal fullerides.

MA 14.8 Tue 12:30 H 1058

**Frustrated magnetism in novel layered Mott insulators.** — •Sergii Grytsiuk[1], Mikhail I. Katsnelson[1], Erik G.C.P. van Loon[2], and Malte Rösner[1] — [1]Institute for Molecules and Materials, Radboud University, Heijendaalseweg 135, 6525AJ Nijmegen, The Netherlands — [2]NanoLund and Division of Mathematical Physics, Physics Department, Lund University, Sweden

Via ab initio down folding, we show that the layered van der Waals distorted kagome compounds $Nb_3X_8$ (X=Cl, Br, and I) are Mott insulators. We demonstrate that the monolayer of these compounds has a frustrated triangular AFM order, while in bulk, an intriguing interplay between intra- and interlayer AFM coupling promotes magnetic frustration further. We show that this leads to chiral in-plane spiralisation of frustrated triangular AFM order at high temperatures and strong collinear interlayer AFM coupling at low temperatures. Furthermore, we explain the "mystic" magnetic phase transition and the nature of the putative "non-magnetic" phase at low temperatures observed in Nb3Cl8, which has not been explained theoretically until now. Finally, our finding offers new opportunities for controlling such non-trivial frustrated magnetism in these layered Mott insulators via doping or substrate screening.

**Invited Talk** MA 14.9 Tue 12:45 H 1058

**New Frontiers in Artificial Spin Ice: Phase Transitions in Two and Three Dimensions** — •Gavin M. Macauley[1,2], Luca Berchialla[1,2], Aleksandra Pac[1,2], Tianyue Wang[1,2], Armin Kleibert[3], Valerio Scagnoli[1,2], Peter M. Derlet[4], and Laura J. Heyrderman[1,2] — [1]Laboratory for Mesoscopic Systems, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Laboratory for Multiscale Materials Experiments, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [3]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [4]Condensed Matter Theory Group, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Artificial spin ices are arrays of strongly correlated nanomagnets, which are coupled through the dipolar interaction. While originally envisaged as a two-dimensional analogue to frustrated rare-earth pyrochlores, they are now studied since they exhibit behaviour such as glassiness and charge fragmentation, and topologically induced textures such as magnetic ‘monopoles’ [1]. In this talk, I will introduce artificial spin ice and discuss some recent work performed in the Laboratory for Mesoscopic Systems. By way of example, I will discuss how they can be used as a platform to study phase transitions by focusing on the example of a rotated kagome-like lattice in two-dimensions and an artificial spin ice based on the buckyball in three-dimensions. These systems have complex phase diagrams, with crossovers, phase transitions, and phase coexistence. [1] Skjaervo, S.H., Marrows, C.H., Stamps, R.L. and Heyderman, L.J. Nat. Rev. Phys. 2, 13-28 (2020).