MA 27: Frustrated Magnets I

Time: Wednesday 15:00–18:30

Location: H 2013

On the origin of correlated diffuse scattering in the hexagonal manganites — \bullet TARA TOŠIĆ¹, ARKADIY SIMONOV², and NICOLA SPALDIN¹ — ¹Materials Theory, ETH Zürich, Switzerland — ²Disordered Materials, ETH Zürich, Switzerland

Using symmetry analysis, first-principles density functional theory and spin dynamics, we pinpoint the origin of the correlated diffuse neutron scattering in hexagonal yttrium manganite (h-YMnO₃). We show that the observed directionality in the structured diffuse scattering in momentum space is a hallmark of the triangular geometry, and that its persistence across a wide range of temperatures, both above and below the Néel temperature, T_N, is a result of the strong magnetic frustration. We argue that excitations away from the magnetic ground state a scenario ruled out in previous modelling attempts - give rise to short-range correlations. Though a hierarchy of nearest-neighbor exchanges and magnetic anisotropy terms, clusters of ordered spins form and interact with each other, creating excitations. We also visualize the magnetic order in terms of composite trimer magnetoelectric monopoles and toroidal moments, rather than individual spins, providing insight into the real space fluctuations, revealing clusters of emerging order in the paramagnetic state, as well as collective shortrange excitations in the ordered Néel phase. Our understanding of this directional diffuse scattering both below and above T_N provides new insight into the magnetic phase transitions in frustrated systems.

MA 27.5 Wed 16:00 H 2013 Superparamagnetic behavior of magnetically frustrated rare earth element substituted R-type hexagonal ferrite suitable for biomedical applications — •IMRAN SADIQ — University of the Punjab, Lahore, Pakistan

This research article reported the inducement of frustration with the substitution of rare earth elements in already frustrated R-type hexagonal ferrites. Crystallographic X-ray diffraction refinement gave the evidence that all the samples display the single phase hexagonal structure with space group P63/mmc. The lattice parameter varied as concentrations increased. The particle sizes measured from TEM and HR-TEM was found to vary in the range of 10-15 nm. These nanoparticles are spherical in shape and exhibit single magnetic domain. The particle size is an excellent agreement with the crystalline size. VSM results revealed its superparamagnetic nature. This frustration turned the magnetic phase of the material from ferrimagnetic to superparamagnetic. It does not have appreciable magnetic hysteresis loop due to zero coercivity and have a negligible values of remanence and squareness ratio revealed its single magnetic domain. The hysteresis loops were fitted theoretically using Langevin function and were in good agreement with experimental results. These materials with almost negligible intrinsic magnetization are suitable for biomedical application especially targeted drugs delivery.

MA 27.6 Wed 16:15 H 2013

Frustrated triangular magnetism in new copper based single crystals — •Aswathi Mannathanath Chakkingal¹, Chloe Fuller Fuller², DMITRY CHERNYSHOV², MAXIM AVDEEV³, MAREIN CHRISTOPHER RAHN¹, YIRAN WANG⁴, FALK PABST⁴, THOMAS DOERT⁴, DARREN PEETS¹, and DMYTRO INOSOV¹ — ¹IFMP, TU Dresden, Germany — ²ESRF, Grenoble, France — ³ANSTO, Sydney, Australia — ⁴Professur f. Anorganische Chemie II, TU Dresden, Germany

The hydrothermal technique is an efficient strategy to synthesize mineralogically inspired structures, including natural and synthetic cuprate minerals with a variety of exciting frustrated magnetic lattices. We report the hydrothermal synthesis of single crystals of a new material $Cu_4(SO_4)(OH)_6$. Single-crystal x-ray and neutron diffraction studies performed to determine the crystal structure reveal the presence of three copper layers which stack in an ABACABAC pattern in the crystal, which results in a large *b* lattice constant of 25Å. Distorted and expanded SO_4^{2-} tetrahedra are identified in the system, likely due to vacancies. The Cu^{2+} copper ions are arranged in buckled sheets consisting of ribbons of edge-sharing and corner-sharing octahedra, and form a heavily distorted triangular lattice. Diffuse scattering measured with synchrotron x-rays also reveals strong stacking-fault disorder in this system. We report details of the crystal structure and its low temperature magnetic properties.

MA 27.1 Wed 15:00 H 2013 Spin-wave dynamics in rouaite, $Cu_2(NO_3)(OD)_3 - \bullet$ DMYTRO S. INOSOV¹, ASWATHI M. CHAKKINGAL¹, ANTON A. KULBAKOV¹, J. ROSS STEWART², and DARREN C. PEETS¹ - ¹Institut für Festkörperund Materialphysik, Fakultät Physik, TU Dresden - ²ISIS neutron source, Rutherford Appleton Laboratory, UK

 $Cu_2(NO_3)(OH)_3$ (mineral name: rouaite) is a quasi-1D quantum spin system with structural similarity to botallackite, in which spinonmagnon mixing has recently been reported by H. Zhang *et al.* [Phys. Rev. Lett. **125** (2020), 037204]. It contains highly distorted triangular-lattice layers composed of alternating ferro- and antiferromagnetic spin- $\frac{1}{2}$ chains. The magnetic excitation spectrum of synthetic deuterated $Cu_2(NO_3)(OD)_3$ single crystals, measured by inelastic neutron scattering, reveals collective excitations with magnon bandwidths of ~11, 1.3 and 0.05 meV in the intrachain, interchain and interlayer directions, respectively, and a spin gap of 0.2 meV. This suggests a hierarchy of exchange interactions at the boundary between quasi-1D and quasi-2D spin systems: While interchain interactions are apparently sufficient to suppress the spinon continuum, some spin-wave branches still show anomalous broadening, reminiscent of the fractionalized behavior in 1D spin chains.

MA 27.2 Wed 15:15 H 2013 Raman scattering of spin- $\frac{1}{2}$ mixed dimensionalities antiferromagnet: α -Cu₂V₂O₇ — • ARVIND KUMAR YOGI¹, HEMANT SINGH KUNWAR¹, ISHA ISHA¹, BINOY KRISHNA DE¹, VIVEK DWIJ², Mayanak Kumar Gupta³, R. Mittal³, R. Venkatesh¹, R. J. Chaudhary¹, Mahesh Vedpathak⁴, and V. G. Sathe¹ — ¹UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India — ²Department of Condensed Matter Physics and Material Science, Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai-400005,India ³Solid State Physics Division, Bhabha Atomic Research Centre, Trombey, Mumbai-400005, India — ⁴Department of Physics, Vidya Pratishthan's Arts, Science and Commerce, Baramati-413133, India We present a detailed investigation of the lattice vibrations and magnetic properties of the spin- $\frac{1}{2} \alpha$ -Cu₂V₂O₇ system by means of x-ray diffraction (XRD), magnetic susceptibility, specific heat, x-ray absorption spectroscopy (XAS), x-ray photoelectron spectroscopy (XPS), and Raman scattering measurements along with a phonon structure calculations by density-functional theory (DFT). Thermodynamic measurements show a long-range ordered (LRO) state at Néel temperature $T_N \sim 33.4 \,\mathrm{K}$. The spin-lattice coupling constant of spin- $\frac{1}{2} \alpha$ -Cu₂V₂O₇ has been calculated for various phonon modes. Despite exchange coupling in 1D chains, the susceptibility, low-temperature heat-capacity and Raman spectroscopic analysis confirms the antiferromagnetic order emerges from the mixed dimensionality nature of the exchange couplings.

MA 27.3 Wed 15:30 H 2013

Emergent quantum criticality in an Ising spin-1/2 zigzag chain antiferromagnet: CaCoV₂O₇ — •ARVIND KUMAR YOGI¹, KOUSHIK CHAKRABORTY¹, ISHA ISHA¹, A. K. BERA², and M. ISOBE³ — ¹UGC-DAE Consortium for Scientific Research, Indore-452001, India — ²Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India — ³Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

We report on a quantum critical behavior in the quasi-1D spin-1/2 zigzag frustrated chain antiferromagnet CaCoV₂O₇, induced by an applied magnetic field. Below $T_N = 3.3$ K our zero-field neutron diffraction studies reveled the up-up-down-down spin structure, stabilized by an order-by-disorder phenomenon. At base temperature, the magnetic order is suppressed by an applied magnetic field (B), inducing a transition into a quantum paramagnetic state at $B_c = 3$ T, as revealed by both neutron diffraction and ESR data. The transition exhibits an unusually sharp phase boundary with the critical exponent $\phi = 0.164(3) \approx 1/6$, in contrast to the earlier experimental observations for uniform spin-1/2 chain systems. Such a sharp QPT is anticipated due to the spin frustration arising from the competing NN and NNN exchange interactions J_1 and J_2 of the zigzag spin chain.

MA 27.4 Wed 15:45 H 2013

 $\label{eq:main_state} MA \ 27.7 \ \ Wed \ 16:30 \ H \ 2013$ Investigation of the magnetoelectric and magnetoelastic properties of the quantum spin liquid candidate Na2Co2TeO_6 — •VILMOS KOCSIS¹, SVEN LUTHER², NICOLÁS PÉREZ¹, WEILIANG YAO³, HANNES KÜHNE², ANJA U. B. WOLTER¹, YUAN LI³, and BERND BÜCHNER¹ — ¹IFW-Dresden, Dresden, Germany — ²HZDR, Dresden, Germany — ³Peking University, Bejing, China

Due to the promising features for quantum computing technologies, the exactly solvable Kitaev model with its bond-dependent interactions has attracted large attention in the scientific community. However, so far there is no such real crystalline material which provides a purely bond-dependent realization of the Kitaev model, as all candidate materials have significant exchange interactions and long-range magnetic order as a result. While these direct exchange interactions are undesirable, they also offer unique possibilities to suppress the long-range order. As an example, the magnetoelastic coupling in some Heisenberg-Kitaev magnets is suggested to be used to suppress the long-range AFM order via uniaxial stress. Here we discuss the magnetoelastic and magnetoelectric properties of the quantum spin liquid candidate Na₂Co₂TeO₆. We study the phase diagram of Na₂Co₂TeO₆ using thermodynamic, magnetic, magnetoelastic, and magnetoelectric measurements. We find strong magnetoelastic and moderate magnetoelectric response responses, magnetostriction is particularly strong for in-plane fields. We contemplate the possibility of using magnetoelectricity in Heisenberg-Kitaev magnets as a new, unique way to extinguish the unwanted long-range order.

15 min. break

MA 27.8 Wed 17:00 H 2013

Frustrated triangular magnetism in new copper based single crystals — •Aswathi Mannathanath Chakkingal¹, Chloe Fuller Fuller², DMITRY CHERNYSHOV², MAXIM AVDEEV³, MAREIN CHRISTOPHER RAHN¹, YIRAN WANG⁴, FALK PABST⁴, THOMAS DOERT⁴, DARREN PEETS¹, and DMYTRO INOSOV¹ — ¹IFMP, TU Dresden, Germany — ²ESRF, Grenoble, France — ³ANSTO, Sydney, Australia — ⁴Professur f. Anorganische Chemie II, TU Dresden, Germany

The hydrothermal technique is an efficient strategy to synthesize mineralogically inspired structures, including natural and synthetic cuprate minerals with a variety of exciting frustrated magnetic lattices. We report the hydrothermal synthesis of single crystals of a new material $Cu_4(SO_4)(OH)_6$. Single-crystal x-ray and neutron diffraction studies performed to determine the crystal structure reveal the presence of three copper layers which stack in an ABACABAC pattern in the crystal, which results in a large *b* lattice constant of 25Å. Distorted and expanded SO_4^{2-} tetrahedra are identified in the system, likely due to vacancies. The Cu^{2+} copper ions are arranged in buckled sheets consisting of ribbons of edge-sharing and corner-sharing octahedra, and form a heavily distorted triangular lattice. Diffuse scattering measured with synchrotron x-rays also reveals strong stacking-fault disorder in this system. We report details of the crystal structure and its low temperature magnetic properties.

MA 27.9 Wed 17:15 H 2013 Towards a diagrammatic approach to quantum spins —

•BJÖRN SBIERSKI — Universität Tübingen, Germany Frustrated quantum spin systems in high dimension are one of the

central challenges for numerical approaches to quantum many body physics. In this situation a diagrammatic approach based on a pseudofermion or pseudo-Majorana spin representation and resummation by the functional renormalization group have provided useful results. However, as two fermions are required to form a single spin operator, this approach lacks efficiency and cannot access spin correlators beyond the two-point object. We present progress towards an alternative diagrammatic approach that directly works with correlation functions of spin operators without any intervening representation of the latter and can also deal with arbitrary spin length S. We discuss the basic diagrammatic rules, definition of vertex ireducibility and various resummation schemes. We present benchmarks of this method and also study spin Hamiltonians of current relevance.

MA 27.10 Wed 17:30 H 2013

Magnetic interaction and anisotropy in frustrated $GdInO_3$ probed by electron spin resonance spectroscopy — •Luca BISCHOF¹, RAHEL OHLENDORF¹, NING YUAN¹, HANS-ALBRECHT KRUG VON NIDDA², and RÜDIGER KLINGELER¹ — ¹Kirchhoff Institute for Physics, Heidelberg University, Germany — ²Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany

Rare earth (R) ions on a triangular lattice as in the ferroelectric RInO₃ have recently emerged as a great possibility to study the physics of magnetically frustrated systems. Here we report X- and Q-band electron spin resonance spectroscopy probing the spin-only magnetism of single-crystal [1] gadolinium indate GdInO₃. Temperature- and angle-dependence of the observed paramagnetic resonance reveal anisotropic magnetic behavior of the system. We find weak single-ion anisotropy ($|D| \approx 4$ GHz) of the Gd-spins using a combined line-width analysis of angular dependencies in X- and Q-band data under consideration of the 10/3-effect. Our data further allow us to quantify the strength of dipolar and isotropic exchange interactions showing that the latter dominantly governs the spin dynamics in GdInO₃.

[1] N. Yuan et al., Phys. Rev. B 108, 224403 (2023).

MA 27.11 Wed 17:45 H 2013 **Constructing Emergent U(1) Symmetries in the Gamma- Prime model** — •SAGAR RAMCHANDANI¹, SIMON TREBST¹, and CIARÁN HICKEY^{1,2,3} — ¹Institute for Theoretical Physics, University of Cologne — ²School of Physics, University College Dublin, Belfield, Dublin — ³Centre for Quantum Engineering, Science, and Technology, University College Dublin

Frustrated magnets can elude the paradigm of spontaneous symmetry breaking and exhibit emergent symmetries at low temperatures. Here we study such an emergent symmetry in a classical spin model whose underlying Hamiltonian actually has very little symmetry, a bond-directional, off-diagonal exchange model inspired by the microscopics of spin-orbit entangled materials (the Gamma-prime model). Surprisingly, the ground state possesses an emergent, continuous U(1) symmetry for a wide variety of lattice geometries with triangular motifs, such as the kagome or hyperkagome lattices. We discuss a thermal order-by-disorder effect which leads to the formation of a Z₆ symmetric phase at the lowest temperatures. Using Monte Carlo simulations, we explore the model's full finite temperature phase diagram and connect its dependence on spatial dimension (2d versus 3d) to known renormalization group results. Finally we comment on the fate of the model in the quantum spin-1/2 limit.

MA 27.12 Wed 18:00 H 2013 Magnetism in the 3D face-centred frustrated spin- $\frac{5}{2}$ system MnSn(OH)₆ — •KAUSHICK K. PARUI¹, ANTON A. KULBAKOV¹, ROMAN GUMENIUK², MAXIM AVDEEV^{3,4}, DARREN C. PEETS¹, and DMYTRO S. INOSOV¹ — ¹IFMP, Technische Universität Dresden, 01069 Dresden, Germany — ²Institut für Experimentelle Physik, TU Bergakademie Freiberg, 09596 Freiberg, Germany — ³ANSTO, Lucas Heights, NSW 2234, Australia — ⁴School of Chemistry, The University of Sydney, Sydney 2006, Australia

Manganese tin hydroxide, $MnSn(OH)_6$ is an A-site-vacant double perovskite with the general stoichiometry $\Box_2(BB')(OH)_6$, where B and B' are transition metals. Here, the magnetic Mn^{2+} ions sit on a facecentred sublattice, which makes the system frustrated and is expected to exhibit exotic magnetism. The structure is characterized by the presence of alternating corner-linked $[Mn^{2+}(OH)_6]$ and $[Sn^{4+}(OH)_6]$ octahedra. Our magnetization measurements reveal the Curie-Weiss temperature of -5.13(1) K, indicating antiferromagnetic interactions, and a paramagnetic moment of $\approx 5.6\mu_{\rm B}$. Despite that, specific heat measurements do not show any sharp magnetic transitions down to 350 mK. This suppression of the magnetic order hints towards a large frustration factor >10. We also report the results of neutron diffraction measurements down to 20 mK and structure refinements based on x-ray and neutron powder diffraction data.

MA 27.13 Wed 18:15 H 2013 Higher-order exchange driven noncoplanar magnetic state and large anomalous Hall effects in kagome magnet — •CHARANPREET SINGH^{1,2}, SK JAMALUDDIN², ASHIS K. NANDY², MASASHI TOKUNAGA³, MAXIM AVDEEV⁴, and AJAYA K. NAYAK² — ¹Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — ²School of Physical Sciences, National Institute of Science Education and Research, Jatni-752050, India — ³The Institute for Solid-State Physics, University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba, 277-8581, Japan — ⁴Australian Nuclear Science and Technology Organisation, New Illawarra Road, Lucas Heights, New South Wales 2234, Australia The noncollinear kagome antiferromagnet Mn_3Sn breaks time reversal symmetry due to the cluster octupole order present in this system. We show that electron doping can induce a noncoplanar magnetic state in Mn_3Sn , which is driven by higher-order exchange interactions and confirmed by our neutron diffraction measurements. The resultant noncoplanar state exhibits a highly tunable scalar spin chirality (SSC) and generates a unique anomalous Hall signal, distinct from the previously examined octupole order-induced Hall signal in this sample. This introduces a novel dual-order phenomenon, where both cluster octupole order and SSC independently contribute to distinct Hall signals. Importantly, the independent manipulation of these orders is demonstrated. Our results open up new possibilities to explore phenomena associated with multiple orders in frustrated magnets.