American Conference on Neutron Scattering

Hard Condensed Matter

* Invited Paper

SESSION B02.01: Magnetic Interaction in Rare Earth Magnets

B02.01.01*
Quantum Disorder and Unconventional Magnetism in ARO_2 (A=Alkali Metal, R=Rare Earth Metal)
Stephen D. Wilson; University of California, Santa Barbara, United States

Triangular lattice compounds decorated with anisotropic J_{eff}=1/2 moments have received revitalized interest due to experimental reports of quantum disordered ground states in classes of layered materials such as $YbMgGaO_4$ [1], $NaYbO_2$ [2], $Ba_8CoNb_6O_{24}$ [3] and other related compounds. Among these, a series of Yb-based compounds of the form $NaYbX_2$ (X=O, S, Se) have emerged as structurally ideal platforms featuring J_{eft}=1/2 Yb moments that derive from well-isolated Kramers crystal-field doublets. A broad spectrum of these systems fail to establish static magnetic order, despite an enhanced exchange field due to relatively close Yb-Yb distances. Uniquely, these materials can also be driven into an intermediate, fluctuation-driven antiferromagnetic state under modest, accessible magnetic fields. This opens the phase boundary between native quantum disorder and fluctuation-driven order to experimental exploration with neutron scattering and other techniques. In this talk, I will present our work in $NaYbO_2$ exploring the magnetic ground state as well as its evolution into a collinear *up-up-down* state under applied magnetic field. I will also discuss some our recent work studying related ARO_2 compounds with alternative R-site species and structure-types. The goal will be to illustrate the spectrum of unconventional magnetic states realized across this class of materials as the R-site cation and lattice symmetries are tuned.

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[2] Bordelon, Mitchell M., Eric Kenney, Chunxiao Liu, Tom Hogan, Lorenzo Posthuma, Marzieh Kavand, Yuanqi Lyu et al. "Field-tunable quantum disordered ground state in the triangular-lattice antiferromagnet NaYbO 2." Nature Physics 15, no. 10 (2019): 1058-1064.
[3] Rawl, R., L. Ge, H. Agrawal, Y. Kamiya, CR Dela Cruz, Nicholas P. Butch, X. F. Sun et al. "Ba 8 CoNb 6 O 24: A spin-1/2 triangular-lattice Heisenberg antiferromagnet in the two-dimensional limit." Physical Review B 95, no. 6 (2017): 060412.

B02.01.02
A Novel Strongly Spin-Orbit Coupled Quantum Dimer Magnet—$Yb_2Si_2O_7$
Gavin L. Hester[1], Harikrishnan S. Nair[1], Timothy R. Reeder[1], Danielle Yahne[1], Tim DeLazzer[1], Leo Berges[2], Djamel Ziat[2], James R. Neilson[1], Adam Aczel[3], Gabriele Sala[3], Jeff Quilliam[2] and Kate Ross[1,4]; [1]Colorado State University, United States; [2]Université de Sherbrooke, Canada; [3]Oak Ridge National Laboratory, United States; [4]CIFAR, Canada

The quantum dimer magnet (QDM) is the canonical example of quantum magnetism. The QDM state consists of entangled nearest-neighbor spin dimers and often exhibits a field-induced triplon Bose-Einstein condensate (BEC) phase. Many compounds based on 3d magnetic cations (Cu^{2+}, Ni^{2+}) have been found that exhibit a quantum dimer state with a BEC phase. Due to the energy scales of 3d magnetism, the critical fields of previous QDM systems with a BEC phase are often above the common field capabilities

at neutron sources (~15 T). We have found a new QDM in the strongly spin-orbit coupled, distorted honeycomb lattice material $Yb_2Si_2O_7$ which exhibits a "dome" of field-induced magnetic ordering in the field vs. temperature phase diagram, reminiscent of a BEC phase, with exceptionally low critical fields of $H_{c1} \sim 0.4$ and $H_{c2} \sim 1.4$ T. Our single crystal neutron scattering, specific heat, and ultrasound velocity measurements reveal a gapped singlet ground state at zero field with sharp, dispersive excitations and an absence of magnetic ordering. Using inelastic neutron scattering in an applied magnetic field we observe a Goldstone mode (gapless to within 0.037 meV) that persists throughout the entire field induced magnetically ordered phase, suggestive of the spontaneous breaking of U(1) symmetry expected for a triplon BEC. However, in contrast to other well-known cases of this phase, the high-field ($\mu_0 H \geq 1.2$ T) part of the phase diagram in $Yb_2Si_2O_7$ is interrupted by an unusual regime signaled by a change in the field dependence of the ultrasound velocity and magnetization, as well as the disappearance of a sharp anomaly in the specific heat. Inelastic neutron scattering data obtained in the high-field regime ($\mu_0 H = 3$ T) was fit using linear spin wave theory as implemented by the Matlab package, SpinW. Contrary to the expectations for a highly spin-orbit coupled compound, the fit indicates that $Yb_2Si_2O_7$ exhibits predominantly isotropic (Heisenberg) exchange. This adds $Yb_2Si_2O_7$ to the growing roster of Yb-based compounds that exhibit dominant Heisenberg exchange. Our measurements provide the opportunity to further study how predominantly isotropic exchange develops in a strongly spin-orbit coupled system and to bring the full power of neutron scattering to bear on the entire phase diagram of a BEC compound.

B02.01.03
Q-Dependent Kondo Spin Fluctuations and a 4*f*/Phonon Resonance in the Intermediate Valent Compound $YbAl_3$
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The intermediate valence (IV) compound $YbAl_3$ exhibits nonintegral valence (Yb $4f^{14-n}f(5d6s)^z$ where $z = 2+n_f = 2.75$) in a moderately heavy ($m^* \sim 20\text{-}30 m_e$) ground state with a large Kondo temperature ($T_K \sim 600$K). We have measured a single crystal of this material on the ARCS spectrometer at the Spallation Neutron Source. We find that at low temperature, the Kondo-scale spin fluctuations have a momentum (**Q**) dependence similar to that seen recently in the IV compound $CePd_3$ and which can be attributed to particle-hole excitations in a coherent itinerant 4*f* correlated ground state. The **Q**-dependence disappears as the temperature is raised and the 4*f* electron bandstates become increasingly incoherent. The measured phonons can be described adequately by a calculation based on standard band theory, without recourse to 4*f* correlations. A low temperature magnetic peak at ~ 30meV shows dispersion identical to an optic phonon branch. This 4*f*/phonon resonance disappears as the temperature is raised. The phonons appear to remain unaffected by the resonance. We speculate that this unusual excitation arises from the large amplitude beating of the light Al atoms against the heavy Yb atoms, resulting in an oscillation of the 4*f*/3*p* hybridization that underlies the heavy fermion physics.

B02.01.04
Crystal Field Splitting and Spin Hamiltonian of the Quantum Magnet $YbCl_3$
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$YbCl_3$ is a nearly ideal honeycomb lattice quantum magnet. We have studied $YbCl_3$ with a combination of neutron scattering, magnetic susceptibility, and heat capacity measurements. We determine the crystal field Hamiltonian through simultaneous refinements of the inelastic neutron scattering and magnetization data. The ground state doublet of the crystal field Hamiltonian is well isolated and results in an effective spin-1/2 system with local easy plane anisotropy at low temperature. The low energy excitation spectrum reflecting the collective properties of $YbCl_3$ shows strong quantum effects which can be explained by a spin wave theory on an ideal honeycomb lattice. In particular, we are able to identify and explain a novel sharp multimagnon feature occurring atop the multimagnon continuum.

B02.01.05
Magnetic Short-Range Correlations and Continuous Transitions in $TmMgGaO_4$
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Young University, United States

The rare-earth triangular antiferromagnet $RMgGaO_4$ is an exciting platform for quantum magnet studies. For R = Yb, experiments have evidenced a spin-liquid-like behavior at low temperature whose origin is still under debate. For R=Tm, the system is a promising candidate to realize transverse Ising model based on non-Kramers Tm^{3+} ion and an effective transverse field originating from crystal electric field. Recent theoretical work has predicted two continuous Kosterlitz-Thouless (KT) transitions at 4 K and 1 K, respectively. Using AC susceptibility, neutron diffraction, and magnetic pair-distribution function measurements, we unveil the two broad transitions in $TmMgGaO_4$ from analysis of scattering results in momentum- and real-space, respectively. We found that short-range three-sublattice magnetic correlations develop over a broad temperature range while cooling and eventually concentrate into quasi-long-range magnetic Bragg peaks at the K-point of the triangular Brillion zone. Furthermore, our data suggests that the local structural disorder that is inescapable in the $RMgGaO_4$ structure, plays a minimal role in the zero-field limit, but strongly affect the collective magnetism under external magnetic fields.
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B02.01.07
Scattering Signatures of Bond-Dependent Magnetic Interactions
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Bond-dependent interactions can generate exotic topological states such as Kitaev and frustrated spin liquids [1,2]. Materials that realize such states have potential applications for topological quantum computation, and are of fundamental interest because they can show entangled ground states whose excitations have fractional quantum numbers [3,4]. Experimentally determining the values of bond-dependent interactions is key to identifying the most promising topological materials. However, such interactions are challenging to measure, for two main reasons [5]. First, most experiments are sensitive only to a subset of the key interactions. Second, current data-analysis approaches typically assume a state with conventional long-range magnetic order — e.g., to model magnon spectra [6,7] — but this requirement is problematic because conventional magnetic ordering is not expected in topological states [4]. In this talk, I explore the extent to which bond-dependent interactions can be extracted from magnetic neutron-diffraction patterns measured in the *paramagnetic* phase. I proceed by simulating diffraction data for a range of bond-dependent models (test cases) on triangular and honeycomb lattices [8]. I show that simulated paramagnetic neutron-diffraction data contain distinctive signatures of the signs of bond-dependent interactions, which can therefore be "read" directly from the data. I further demonstrate that, in every test case, values of the bond-dependent interactions can be accurately determined *via* unconstrained fits, and that this approach is robust to the level of statistical noise typical of real measurements. Perhaps most surprisingly, powder averaging does not entirely remove this sensitivity to bond-dependent interactions; consequently, powder-diffraction data can constrain such interactions when single-crystal samples are unavailable. I conclude by discussing the advantages, limitations, and possible applications of this approach, and discuss my results in the context of developments in reverse Monte Carlo refinement [9], pair distribution function analysis [10], and machine learning [11].

[1] Kitaev, *Ann. Phys.* **303**, 2 (2003); [2] Zhu *et al.*, *Phys. Rev. Lett.* **120**, 207203 (2018); [3] Takagi *et al.*, *Nat. Rev. Phys*. **1**, 264 (2019); [4] Broholm *et al.*, *Science* **367**, eaay0668 (2020); [5] Laurell and Okamoto, *npj Quantum Mater.* **5**, 2 (2020); [6] Banerjee *et al.*, *Nat. Mater.* **15**, 733 (2016); [7] Ran *et al.*, *Phys. Rev. Lett.* **118**, 107203 (2017); [8] Chaloupka and Khaliullin, *Phys. Rev. B* **92**, 024413 (2015); [9] Paddison and Goodwin, *Phys. Rev. Lett.* **108**, 017204 (2012); [10] Frandsen, Yang, and Billinge, *Acta Crystallogr. A* **70**, 3 (2014); [11] Samarakoon *et al., Nat. Commun.* **11**, 892 (2020).

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SESSION B02.02: Perovskites and Related Materials

B02.02.01*
Electrolyte-Gate-Controlled Magnetism in Perovskite Oxides Probed by *Operando* Polarized Neutron Reflectometry
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Yu[1], Guichuan Yu[1], Martin Greven[1], Peter Orth[6], Rafael Fernandes[1], Boris Shklovskii[1], Turan Birol[1], Zhan Zhang[7], Hua Zhou[7], John W. Freeland[7] and Chris Leighton[1]; [1]University of Minnesota, United States; [2]Augsburg University, United States;
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[5]The University of Tennessee, Knoxville, United States; [6]Iowa State University, United States; [7]Argonne National Laboratory, United States

Recently, incorporation of electrolytes such as ionic liquids into field-effect transistors has enabled electric double layer transistors (EDLTs) capable of inducing very large (up to 10^{15} cm^{-2}) charge carrier densities at surfaces. This correspond to significant fractions of an electron or hole per unit cell in most materials, sufficient to *electrically control* electronic/magnetic phase transitions. While this has stimulated great interest, many challenges remain, including understanding the true mechanisms (*i.e*., electrostatic *vs*. electrochemical [1]), developing *operando* characterization methods, and assessing the full power and universality of the approach. Here, I will present our recent work applying electrolyte gating using solid ion gels [1-6] to magnetic complex oxides (*e.g*., $La_{1-x}Sr_xCoO_{3-\delta}$), focused on electrical control of magnetism, probed *via operando* polarized neutron reflectometry (PNR). Our findings greatly clarify the issue of electrostatic *vs*. electrochemical response, culminating in a picture where electrostatic gating *vs*. oxygen vacancy creation/annihilation can be understood and predicted based on bias polarity, and the enthalpy of formation and diffusivity of oxygen vacancies [1-6]. Critically, this was achieved *via* development of *operando* probes, particularly PNR [3,6], synchrotron X-ray diffraction [3], and X-ray absorption spectroscopy/magnetic circular dichroism (XAS/XMCD) [4]. Most significantly, electrical control of the Curie temperature in $La_{1-x}Sr_xCoO_{3-\delta}$ has been demonstrated over a ~200 K window by an electrochemical mechanism [3] and over a record 160 K window by electrostatic gating [6]. In both cases PNR has been used as an *operando* probe of the electrically-controlled ferromagnetism, generating insight far beyond transport alone.
Work supported by the US Department of Energy through the University of Minnesota Center for Quantum Materials.

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[2] J. Walter, H. Wang, B. Luo and C. Leighton, *ACS Nano* **10**, 7799 (2016).
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B02.02.02*
Tuning Chemical Short Range Order in the Solid State
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It is widely recognized in catalysis, energy storage and conversion, and a wide array of other functional materials areas that unique properties and characteristics are governed by intricate structural-chemical relationships. Locally ordered cation and anion motifs offer a gamut of possibilities but remain a challenge because experimental tools to observe them are limited. We present recent efforts to apply and extend neutron and X-ray total scattering and related probes to explore *chemical short range order* and associated structure-property responses in solid state materials. First, we will present our work uncovering universal B-site cation ordering in mixed metal inverse spinel oxides, materials of interest as high voltage cathodes in Li-ion batteries. It is found that the degree and length-scale of cation order depend on the charge and ionic radii difference between constituents, unifying the view of many observed physical properties in the structural archetype. Ongoing efforts to increase the reversibility of charge-discharge chemistries will be described. Second, we will present structure-property characteristics of pyrochlore $Ln_2M_2O_7$ materials, a new family in the emerging class of high entropy oxides (HEOs). HEOs exhibit a single-phase crystal structure containing five or more different metal cations of the same amount on single crystallographic lattice sites. The resulting configurational disorder promises unique property characteristics, such as increased structural stability (by impairing the migration of defects) and multi-functional "cocktail" effects (through high numbers of possible element combinations and their interactions). We combine numerous local structure probes and a complex modeling framework to explore the characteristics that specific participating cations and synthesis conditions impart to the family, demonstrating a rich tunability of associated properties. These examples highlight a broader theme of our research aimed at

extracting crystal structure models from experimental data with the detail needed to guide and validate solid state theories, and design new and improved functional materials. Current challenges and future opportunities in this arena will be discussed.

B02.02.03
Diffuse Neutron and X-Ray Scattering from Cesium Lead Bromide
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Cesium lead bromide has attracted recent attention, along with other lead halide perovskites, due to its optoelectronic properties. It has been proposed that the long carrier lifetime supporting these properties is due to local structural fluctuations. To investigate the short-range lattice distortions that such fluctuations would imply, diffuse neutron and x-ray scattering experiments were performed on single crystals of $CsPbBr_3$ across a range of temperatures spanning the two structural phase transitions. Significant diffuse scattering indicating two-dimensional deviations from the average crystals structure was observed in both higher-temperature phases, indicating that local planar distortions remain present at these higher temperatures. Distinct elastic and inelastic features, distinguishing between static and dynamic forms of local displacement correlations, were found in the neutron scattering data collected at CORELLI, with the short-range planar distortions shown to be quasi-static in nature. Models of locally correlated atomic displacements are able reproduce the observed diffuse scattering, emphasizing the importance of local displacement in understanding the structure of this material. This work was supported by the US DOE, Office of Science, Basic Energy Science, Materials Sciences and Engineering Division.

B02.02.04
In Search of Microscopics of Quantum Annealing
Steffen Säubert[1], Colin Sarkis[1], Feng Ye[2] and Kate Ross[1,3]; [1]Colorado State University, United States; [2]Oak Ridge National Laboratory, United States; [3]CIFAR, Canada

Quantum annealing refers to a method for solving optimization problems through quantum fluctuations rather than the more traditional thermal fluctuations and has been argued to produce a speed-up for some complex optimization problems [1]. A model system to study quantum annealing is the transverse field Ising model (TFIM) that is experimentally realized in the tetragonal material LiHoF4 and its disordered variant LiHoxY1-xF4 [2]. The disordered TFIM provides a complex optimization problem, where the ground state of the system can be reached more efficiently by quantum fluctuations that induce tunneling under an applied transverse field. This has already been observed, through ac magnetic susceptometry, in the magnetically diluted form LiHoxY1-xF4 (x=0.44) [3], however, without gaining direct information on the microscopic spin correlations that are involved, i.e. the quantity that is actually being optimized. We report on details of the microscopic spin correlations via a measurement of elastic diffuse magnetic neutron scattering in three dimensions.

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B02.02.05
Realization of the Orbital-Selective Mott State at the Molecular Level in Ba3LaRu2O9
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Molecular magnets based on heavy transition metals have recently attracted significant interest in the quest for novel magnetic properties. For systems with an odd number of valence electrons per molecule, high or low molecular spin states are typically expected in the double exchange or quasi-molecular orbital limits respectively. In this talk, we use bulk characterization, muon spin relaxation, neutron diffraction, and inelastic neutron scattering to identify a rare intermediate spin-3/2 per dimer state that cannot be understood in a double exchange or quasi-molecular orbital picture and instead arises from orbital-selective Mott insulating behavior at the molecular level. Our measurements are also indicative of stripe magnetic order below TN = 25 K for these molecular spin-3/2 degrees-of-freedom, which is consistent with expectations for an ideal triangular lattice with significant next nearest neighbor in-plane exchange. Finally, we present neutron diffraction and Raman spectroscopy data under applied pressure that reveal a coincident crystal symmetry lowering and spin state transition from S = 3/2 to S = 1/2 at a modest pressure of ~ 1 GPa, which

highlights the delicate balance between competing energy scales in this system.

SESSION B02.03: Frustrated Magnets

B02.03.01*
Materializing Rival Ground States in the Barlowite Family of Kagome Magnets
Rebecca Smaha[1,2], Wei He[1,2], Jack M. Jiang[1,2], Jiajia Wen[2], Yi-Fan Jiang[2], John P. Sheckelton[2], Charles J. Titus[1], Suyin G. Wang[3], Yu-Sheng Chen[3], Simon J. Teat[4], Adam Aczel[5,6], Yang Zhao[7,8], Guangyong Xu[7], Jeffrey W. Lynn[7], Hong-Chen Jiang[2] and Young S. Lee[1,2]; [1]Stanford University, United States; [2]SLAC National Accelerator Laboratory, United States; [3]The University of Chicago, United States; [4]Lawrence Berkeley National Laboratory, United States; [5]Oak Ridge National Laboratory, United States; [6]The University of Tennessee, Knoxville, United States; [7]National Institute of Standards and Technology, United States; [8]University of Maryland, College Park, United States

Quantum magnets display exotic phases that may be strongly influenced by small differences in structure and composition. The quantum spin liquid (QSL) is an unusual magnetic ground state, characterized by long-range quantum entanglement of the spins but a lack of long-range magnetic order down to T=0K. This is believed to be possible in highly frustrated spin-1/2 systems, so materials with a kagome arrangement of Cu^{2+} ions are prime candidates. We find that when the bonds of the kagome lattice are modulated with a periodic pattern, new quantum ground states emerge. Newly synthesized crystalline barlowite ($Cu_4(OH)_6FBr$) and Zn-substituted barlowite demonstrate the delicate interplay between singlet states and spin order on the spin-1/2 kagome lattice. Comprehensive structural and magnetic measurements (including single crystal and powder X-ray diffraction, powder neutron diffraction, and single crystal neutron scattering) were performed to address open questions about their crystal and magnetic structures. We reveal a clear structure-properties relationship between two variants of barlowite with distinct low-temperature structures. Our novel single crystalline barlowite has a subtle symmetry lowering, and its kagome lattice contains a motif of distorted and undistorted triangles, for which numerical simulations predict a pinwheel valence bond crystal state instead of a QSL state. The presence of interlayer spins eventually leads to novel pinwheel $q=0$ magnetic order, which we elucidate with single crystal neutron scattering. Recent inelastic and in-field elastic neutron scattering results will also be discussed. Sizable single crystals of QSL candidate Zn-substituted barlowite ($Cu_{3.44}Zn_{0.56}(OH)_6FBr$) were grown for the first time and compared to $Cu_{3.05}Zn_{0.95}(OH)_6FBr$ and herbertsmithite. Significantly, no magnetic transition is observed down to T=0.1K, indicating a surprising robustness of the QSL against interlayer Cu^{2+} impurities. These samples span a spectrum of quantum spin liquidity, allowing this exotic ground state to be probed systematically.

B02.03.02
Emergent Quasi-Spin Anisotropy in Highly Frustrated Pseudobrookite Fe_2TiO_5
P. G. LaBarre[1], Daniel Phelan[2], Y. Xin[3], Feng Ye[4], Daniel M. Pajerowski[4], T. Siegrist[5,3], Stephan Rosenkranz[2] and A. P. Ramirez[1]; [1]University of California, United States; [2]Argonne National Laboratory, United States; [3]National High Magnetic Field Laboratory, United States; [4]Oak Ridge National Laboratory, United States; [5]FAMU-FSU College of Engineering, United States

Magnetic anisotropy is essential for many applications and has recently also been a focal point of fundamental importance as it can play a pivotal role in quantum spin liquids. Such anisotropy originates from the combined effects of orbital occupation, spatial anisotropy, and spin-orbit coupling. In spin glasses, anisotropy is usually considered single-ion-like, that is, it exists independent of spin-spin interactions and anisotropy exists above the freezing temperature. An *s*-state ion of a half-filled shell, such as Fe^{3+}, on the other hand is completely isotropic since it's wave function has no orbital character, though second order effects due to virtual interactions with non-half-filled ions exist. Since for such systems there is expected to be very small, if any, anisotropy, it is surprising that Fe_2TiO_5 exhibits highly anisotropic responses both below and above the spin glass freezing temperature $T_f \sim 55$K. This compound crystallizes in the orthorhombic pseudobrookite structure with close to completely random mixing among Fe^{3+} and Ti^{4+} ions. While attempts to explain the observed Ising-like anisotropy in the susceptibility above T_f and the absence of any freezing anomaly in the plane perpendicular to the Ising axis at T_f were based on the phenomenological introduction of anisotropy, its origin remained unexplained. In order to obtain a detailed understanding of these puzzling observations, we utilized single crystal diffuse and inelastic neutron scattering to investigate in detail the spin correlations. Upon cooling towards the freezing temperature, we observe the growth of streaks of highly anisotropic diffuse magnetic scattering, which evidence the growth of surfboard-shaped regions of

correlated spins: while spins are strongly correlated along an axis perpendicular to the Ising-axis with a correlation length extending over ten unit cells in the spin glass state, along the Ising axis the correlation length is about four times smaller and along the remaining axis, spins are only correlated over one or two nearest neighbors. The comparison of energy-integrated to elastic only scattering shows that substantial fluctuations remain present at the lowest temperature measured, and inelastic measurements indeed reveal spin excitations extending to at least 10meV. We will discuss that these surfboards form nanoscale antiferromagnets that mimic the behavior of an XY spin system, and that the transverse fluctuations of these XY quasi-spins are the "quasi-spin" degrees of freedom that freeze. We therefore suggest that the Ising anisotropy observed in Fe_2TiO_5 is an emergent property, driven by interactions among atomic spins. This work was supported by the US DOE, Office of Science, Basic Energy Science, Materials Sciences and Engineering Division.

B02.03.03
SU(3) Magnetic Excitations of the Frustrated Ising Magnet FeI2
Martin Mourigal; Georgia Institute of Technology, United States

We present a detailed investigation of the spin dynamics in single-crystals of the layered spin-one triangular-lattice compound FeI_2. Previous thermo-magnetic measurements revealed a strong Ising single-ion anisotropy for the Fe2+ ions in FeI2 and a magnetically long-range ordered state below 9.3K, which can be understood from the competition between nearest neighbor ferromagnetic interactions and a complex set of further-neighbor interactions. Early neutron scattering, far-infrared and ESR measurements, revealed the emergence of a two-magnon bound state (TMBS) as the lowest energy mode from this ordered state. The TMBS carries an apparent g-factor that is doubled compared to that of single magnon excitations, which can be explained by a change of 2 units in spin angular momentum, at odds with the dipole selection rule. We revisit the spin excitations of FeI_2 using modern neutron-scattering instrumentation and map out the magnetic structure, diffuse scattering and low-energy magnetic excitation spectrum. We extract a model Hamiltonian for FeI_2 and elucidate a novel hybridization mechanism that quantitatively explains current and previous spectroscopic experiments on this enigmatic compound. The work at Georgia Tech was sponsored by the Department of Energy under DE-SC-0018660.

B02.03.04
The Structure Factor Studies of the Ising Shastry Sutherland Model Revealed Using Quantum Annealing
Arnab Banerjee[1], Paul Kairys[2], Travis Humble[3], Jack Raymond[4] and Andrew King[4]; [1]Purdue University, United States; [2]The University of Tennessee, Knoxville, United States; [3]Oak Ridge National Laboratory, United States; [4]D-Wave Systems, Canada

The macroscopic properties of a material depend on the strengths and symmetries of the microscopic Hamiltonian which can be tuned both by an external stimulus, such as a magnetic field or due to intrinsic disorder. Understanding and tuning the phases of matter and their transitions is in the heart of modern material science. In this theoretical work, we establish a quantum hardware route to understanding phases of materials by successfully computing of the phases of a 468-spin Shastry-Sutherland Hamiltonian on a 2000 qubit D-Wave Quantum Annealer. We formulate a new approach that rely on iterative quantum annealing of a model Hamiltonian to improve computational convergence. We introduce a novel use of mean-field boundary conditions to tune the effects of disorder within the chip to mimic physical disorder in real materials and to mitigate the errors from finite system size. We not only recover four distinct phases predicted by Monte Carlo, including the well-known transition to a fractional magnetization plateau, within a very small number of iterations but also identify the critical behavior at their transitions as well as the effects from disorder. Our results establish quantum annealing to provide a viable and accurate description of the ground state of magnetic Hamiltonians, providing an exciting pathway to understanding data obtained from neutron scattering experiments on real spintronic materials.

B02.03.05
Electric Current Control of the Spin-Orbit Coupled 4*d* Ruthenate $Ca_2Ru_{0.97}Mn_{0.03}O_4$
Feng Ye[1], Christina Hoffmann[1], Hengdi Zhao[2] and Gang Cao[2]; [1]Oak Ridge National Laboratory, United States; [2]University of Colorado Boulder, United States

The unique interplay between spin-orbit interaction (SOI) and Coulomb correlation (U) in *4d*/*5d* oxides drives unusual physical behavior. Novel nonequilibrium phenomena can be further induced by external stimuli including synchrotron x-ray, magnetic field, and electric current [1–3]. In this talk, I will present neutron diffraction study of the quasi-two-dimensional Mott $Ca_2Ru_{0.97}Mn_{0.03}O_4$, which shows dramatic reduction of the electric resistivity, suppression of the antiferromagnetic transition, and induction of new orbital order above critical current

density. Our in-situ structural characterization implies that the in-plane orthorhombicity diminishes with increasing current density, accompanied by the straightened of the Ru-O-Ru bonding angles. The temperature-current phase diagram establishes an intimate correlation between the lattice and electronic structure in this nonequilibrium, steady state driven by current [4]. Our results shed light to the nature of the Mott-Insulator transition and provide key information for the emerging phenomena near the transition.

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SESSION B03.01: Student Research Spotlight

B03.01.01*
Unravelling Competing Microscopic Interactions at a Phase Boundary—A Single Crystal Study of the Metastable Antiferromagnetic Pyrochlore $Yb_2Ge_2O_7$

Colin Sarkis[1], Jeff Rau[2,3], Duminda Sanjeewa[4], Matthew Powell[4], Joseph Kolis[4], Jonathon Marbey[5], Stephen Hill[5], Jose A. Rodriguez-Rivera[6], Harikrishnan S. Nair[1], Michel Gingras[7] and Kate Ross[1]; [1]Colorado State University, United States; [2]University of Windsor, Canada; [3]Max Planck Institute, Germany; [4]Clemson University, United States; [5]Florida State University, United States; [6]National Institute of Standards and Technology, United States; [7]University of Waterloo, Canada

Rare earth pyrochlore oxides have been found to be hosts for a wide breadth of exotic phenomena based on strong frustration. Studies on single crystals of $Yb_2Ti_2O_7$ have established that it forms a ferromagnetic (FM) ground state, but lies near a classical phase boundary between FM and antiferromagnetic (AFM) states. Meanwhile, powder neutron scattering studies of $Yb_2Ge_2O_7$ show it selects an AFM state. Despite this difference, these Yb pyrochlores share the same unusual spin dynamics in zero field, which has been proposed to be a result of phase competition. Further progress has been impeded by inaccessibility of single crystals of $Yb_2Ge_2O_7$. We report inelastic neutron scattering measurements on a co-aligned mosaic of single crystals of $Yb_2Ge_2O_7$ grown by a hydrothermal method. Comparison of field-polarized INS data with linear Spin-wave calculations allowed the determination of the four symmetry allowed exchange parameters for $Yb_2Ge_2O_7$. The *g*-tensor was independently determined from electron paramagnetic resonance on a $Lu_{1.98}Yb_{0.02}Ge_2O_7$ sample in order to enable an unambiguous determination of these parameters. Our analysis and theoretical modeling place $Yb_2Ge_2O_7$ in extreme proximity to the classical phase boundary between the AFM and FM phase, lending strong support to the notion of phase competition as playing a key role in the Yb pyrochlore family. DOE:DE-SC0020071

B03.01.02
Pseudo-Spin Versus Magnetic Dipole Moment Ordering in the Isosceles Triangular Lattice Material $K_3Er(VO_4)_2$

Danielle Yahne[1], Liurukara Sanjeewa[2], Athena Sefat[2], Bradley S. Stadelman[3], Joseph Kolis[3], Stuart Calder[2] and Kate Ross[1,4]; [1]Colorado State University, United States; [2]Oak Ridge National Laboratory, United States; [3]Clemson University, United States; [4]CIFAR, Canada

Spin-½ antiferromagnetic triangular lattice models are the quintessential example of geometric frustration, with the nature of anisotropies in the model revealing a variety of different ground states and quantum effects. Strong spin-orbit coupling and crystal field effects can cause the rare-earth ions to form pseudo-spin-½ magnetic moments with anisotropic single-ion and exchange properties. Thus, rare-earth based triangular lattices are an interesting playground to explore the interplay between frustration and anisotropy. Here we study one such case, the rare-earth double vanadate glaserite material $K_3Er(VO_4)_2$, which is a quasi-2D isosceles triangular antiferromagnet. Our specific heat and neutron powder diffraction data from $K_3Er(VO_4)_2$ reveal a transition to long-range magnetic order at $T_N = 155 \pm 5$ mK, recovering all Rln(2) entropy. A Warren-like Bragg peak profile in addition to 3D ordered Bragg peaks indicates a coexistence of 2D and 3D magnetic correlations below T_N. Our magnetic susceptibility data reveals that Er^{3+} takes on a strong XY single-ion anisotropy in $K_3Er(VO_4)_2$, and therefore should contain the majority of the moment within the ab-plane. Considering this, in conjunction with our neutron powder diffraction data taken below T_N, we find that the 3D ordered magnetic structure consists of b-axis aligned antiferromagnetic layers ($3.55\mu_B$) slightly canted in the c-axis, as well as layers of small antiferromagnetic c-axis aligned moments ($0.72\mu_B$). $K_3Er(VO_4)_2$ provides a clear example of how pseudo-spin-½ ordering can manifest as widely varying magnetic moment sizes depending on the pseudo-

spin orientation, due to *g*-tensor anisotropy.

B03.01.03
Magnetic Properties of the Doped Mott Insulator $YTiO_3$
Joseph Joe[1], Sajna Hameed[1], Peter Gehring[2], Masaaki Matsuda[3] and Martin Greven[1]; [1]University of Minnesota Twin Cities, United States; [2]National Institute of Standards and Technology, United States; [3]Oak Ridge National Laboratory, United States

The transition metal oxides $RTiO_3$, where R is a trivalent rare-earth ion, are typical Mott-Hubbard insulators, with the Ti^{3+} ion in the $3d^1$ configuration. The observed $GdFeO_3$-type tilt distortion of the TiO_6 octahedra controls the electron transfer between the Ti $3d_1$ and O 2p orbitals, and hence constitutes a bandwidth-control mechanism. The end members $YTiO_3$ and $LaTiO_3$ of this series exhibit large and small distortions, respectively, with Ti-O-Ti bond angles of 140° and 156°. The physical properties across the $RTiO_3$ series exhibit significant variation dependent on the rare-earth ion, as $YTiO_3$ is a ferromagnet (FM), whereas $LaTiO_3$ is an antiferromagnet (AFM). In both cases, hole doping induces a metallic state; the insulator-metal transition (IMT) in $Y_{1-x}Ca_xTiO_3$ and $La_{1-y}Sr_yTiO_3$ occurs at wildly different concentrations of x=0.37 and y=0.05, respectively [1]. The robust insulating state of $YTiO_3$ makes the system particularly interesting, notwithstanding various other peculiarities, as it has been argued that orbital order is responsible for the ferromagnetic ground state. Here we report elastic and inelastic neutron scattering results for $Y_{1-x}La_xTiO3$ and $Y_{1-x}Ca_xTiO_3$, with focus on the spin-wave spectrum and magnetic order parameter, in order to elucidate the respective evolution from FM to AFM insulator and FM insulator to paramagnetic metal. The work at the University of Minnesota was funded by the Department of Energy through the University of Minnesota Center for Quantum Materials, under DE-SC-0006858.
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B03.01.04
Influence of Plastic Deformation on the Structural, Transport and Magnetic Properties of Strontium Titanate
Sajna Hameed[1], Damjan Pelc[1], Zachary W. Anderson[1], Richard J. Spieker[1], Marin Lukas[2], Yaohua Liu[3], Matthew J. Krogstad[4], Raymond Osborn[4], Chris Leighton[1] and Martin Greven[1]; [1]University of Minnesota Twin Cities, United States; [2]University of Zagreb, Croatia; [3]Oak Ridge National Laboratory, United States; [4]Argonne National Laboratory, United States

Strontium titanate ($SrTiO_3$, STO) is one of the most important transition metal oxides: it is a model perovskite with a structural phase transition, and also one of the most commonly used single crystal substrates for epitaxial growth of oxide thin films. Superconductivity in STO occurs at unusually low carrier densities at temperatures well below 1 K and is not understood, even five decades after its discovery. Building on our recent work on oxide superconductors [1], we have begun to explore another interesting property of STO: its high ductility at room temperature, which has allowed us to plastically deform single crystals using uniaxial pressure. Using diffuse neutron and X-ray scattering, transport and magnetometry measurements, we have determined the influence of this compressive plastic deformation on the structural, transport and magnetic properties of STO, with particular emphasis on the superconducting state. The results push the limits of superconductivity in low-density electronic systems such as STO, suggest that deformed STO is a potential high-temperature superconductor and, more broadly, demonstrate the feasibility of plastic deformation as a tool to manipulate the electronic properties of quantum materials [2].

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B03.01.06
Local Atomic Correlations in 1T-$TaS_{2-2x}Se_{2x}$ across the CDW Phases
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Studies on transition metal dichalcogenides (TMD) is of great significance due to their interesting topological properties and unusual superconductivity. These materials are prototypical examples of charge density wave (CDW) instability where the CDW state is in close proximity to superconductivity. In this project, we investigate the CDW phases in TaX_2 class of TMDs, where X = S, Se. 1T-TaS_2 has attracted much attention recently because of the possibility of an exotic quantum spin liquid (QSL) state. This is proposed to be one of the few model spin configurations that may harbor a QSL state. 1T-TaS_2 undergoes a series of phase transitions upon cooling and achieves a commensurate CDW (CCDW) phase below 183K. The CCDW transition is accompanied by a periodic lattice distortion. It is

reported that the system forms a √13×√13 super cell, described as a star-of-David, with a large distortion of about 10% of the lattice constant, in the CCDW state. Simultaneously, electron correlation effects set in and localize the unpaired electron at the center of star, leading to a Mott insulating state with S = 1/2 spins arranged in an ideal triangular lattice of 1T-TaS_2. On the other hand, 1T-$TaSe_2$ undergoes CCDW transition at a higher temperature of 473 K and remains metallic upon cooling to low temperatures. No metal-to-insulator transition is observed in 1T-$TaSe_2$ which implies that the spin on the unpaired electron is not localized within the star-of-David and suggests a different distortion is at play. This is interesting given that both 1T-TaS_2 and $TaSe_2$ have trigonal symmetry and undergo similar periodic modulations on CCDW transition. To elucidate the nature of the local atomic correlations upon cooling into the CCDW transition and understand the origin of the differences in TaS_2 and $TaSe_2$, the local atomic structure was obtained by Fourier transforming the synchrotron X-ray diffraction data. In this project, we investigate the local structure and ordering in 1T-TaS_2 and 1T-$TaSe_2$ systems as they undergo the CDW transition by analyzing the atomic pair distribution function (PDF). We also look at low-energy inelastic neutron scattering measurements to study magnetic excitations in this material.

B03.01.07
First Principles Study of the Phonons in an Undoped Insulating Cuprate
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Accurate first-principles modelling of the cuprates is essential to interpreting the results of experiments. However, most previous calculations performed at low doping find a metallic ground state instead of the experimentally determined insulating state. The consequences of this failure are particularly apparent when comparing phonons calculated from the metallic electronic structure to inelastic neutron and X-ray data. Measurements of the Cu-O branch in La_2CuO_4 (LCO) at low doping show very little dispersion across the Brillouin zone, while first principles density functional theory (DFT) calculations show this branch dispersing steeply (which actually agrees better with the overdoped metallic state). However, a recently developed DFT exchange-correlation functional has been shown to accurately predict the insulating electronic structure of LCO. In my talk, I will present the results of phonon calculations performed using this new functional and demonstrate how DFT results can be directly compared to data from inelastic neutron and X-ray experiments. In the case of undoped LCO, we find better agreement than previously reported between the calculated and measured dispersion of the Cu-O bond stretching branch, suggesting that using the correct insulating electronic structure is necessary for accurate first-principles modelling of phonons in the cuprates. *This work was supported by the DOE, Office of Basic Energy Sciences, Office of Science, under Contract No. DE-SC0006939.

B03.01.08
Anomalous Magnetic Structure and Dynamics in $FeGe_2$
Yaokun Su[1], Hillary Smith[2], Matthew Stone[3], Douglas L. Abernathy[3] and Chen Li[1]; [1]University of California, Riverside, United States; [2]California Institute of Technology, United States; [3]Oak Ridge National Laboratory, United States

Inelastic neutron scattering was used to probe order and dynamics in single crystal $FeGe_2$ at 20 and 300 K. An unusual magnetic feature in the dynamical structure factor was found in the HK0 planes. It was found that the anomaly only exists as the dynamic magnetic structure at low temperature, but part of it condenses to the static structure at room temperature. At 300 K, the magnetic anomaly appears to be rods intensity connecting magnetic zone centers along [110] and [1-10]. At 20 K, the rods intensity is detached from the magnetic zone centers to form a dot-dash-dot pattern. This anomaly is far from the magnetic satellites of the incommensurate state. The large discrepancies between experiment and phonon/magnon calculation are attributed to the strong magnon-phonon interactions and it is speculated that they may also be related to the anomaly.

SESSION B03.02: Nanomaterials and Layered Thin-Film

B03.02.01
Using a Combination of Neutron and X-Ray Reflectometry to Reveal Complex Antiferromagnetic Canting Structures in Oxide Heterostructures

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Interface functionality in oxide heterostructures can be controlled by strain engineering, due to the nearly degenerate ground states of competing order in these

systems. A central question is what role structural reconstructions play inestablishing and controlling new magnetic spin textures. In general, probing antiferromagnetic spin structures is difficult but important in new spintronic devices. To address this question, (111)-oriented epitaxial heterostructures of antiferromagnetic (AF) $LaFeO_3$ (LFO) and ferromagnetic $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) is used as model system, and we present data on the interplay between AF spin axis of LFO and the occurrence of magnetic reconstructions at the (111)-oriented LSMO/LFO interface. To probe the spin texture of the different layers, we rely on a combination of soft x-ray spectroscopy, x-ray photoemission electron microscopy and neutron reflectometry. The AF LFO is spin-flopped coupled (perpendicular) to the FM LSMO, however at the interface a canting of the AF spins is induced, resulting in a net moment in the LFO and a spiral spin structure. We show that the AF spin axis in single layers of LFO can be tuned by thickness, crystallographic orientation and strain. Hence, we can by using different substrates induce different types of spiral structures at the interface. We use soft x-ray resonant reflectivity with linear polarized light and spin polarized neutron reflectivity to directly probe the depth dependence on the AF and FM spin axis in these systems. In addition, we can use magnetic fields to change the spiral structure. Due to the magnetic exchange coupling at the interface, the AF spin axis turns/rotates when an applied field aligns the FM spins. Hence, creating systems with a competition between exchange coupling and magneto crystalline anisotropy enables us to control the spin canting in the AF layer.

B03.02.02
Probing Room Temperature Magnetism in Nano-$MnCr_2O_4$ Spinels Using Polarization-Analyzed vSANS
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The spinel chromate $MnCr_2O_4$ is conventionally interesting in that it is magnetoelastic and magneto-dielectric below $T_N = 43$ K and shows ferroelectricity at $T_S = 18$ K with the onset of short-range spiral spin order [1, 2, 3]. However, high temperature magnetic susceptibility (~1000 K) of our ball-milled nanoparticles of 550 $\pm$ 150 nm or 180 $\pm$ 50 nm indicates the presence of spin correlations up to 800 K. To understand the magnetic morphology at remanence (0.007 T) and higher field (1.5 T) at 300 K, we employ the converging beam with high resolution detector option at VSANS (the very Small Angle Neutron Scattering instrument at the NIST Center for Neutron Research), additionally adding full neutron spin polarization analysis involving a super mirror, RF flipper, and He3 spin analyzer. This probes the Q-range of 0.0003 to 0.13 inverse angstroms. Spin-flip scattering indicates that while the magnetism at 0.007 T nearly follows the structural scattering for most of the observable Q-range, but at very low Q below about 0.001 inverse angstroms the magnetic scattering diverges front the structural scattering and quickly drops toward zero intensity, indicative of anti-ferromagnetic alignment between magnetic domains within grains (both samples). Additionally, the difference between DD and UU scattering (or between D and U for half-polarization without the He3 spin analyzer) effectively probes the nuclear-magnetic cross-term. We see an oscillatory negative and positive difference which indicates that the net magnetism parallel to the applied magnetic field is not coherent with the underlying structure for both magnetic field conditions. This difference is larger in magnitude and with a different Q-dependence for the higher field (more detailed modeling in progress). For both samples (180 nm and 550 nm samples) conventional SANS does not reach a sufficiently low Q to observe the magnetic morphologies described; the polarization analysis is additionally needed no observe the magnetic structure that is dominated by the structural scattering contribution.

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Access to vSANS was provided by the Center for High Resolution Neutron Scattering, a partnership between the National Institute of Standards and Technology and the National Science Foundation under Agreement No. DMR-1508249. HSN and AEG acknowledge Rising Stars award from UT and UTEP start-up funds.

B03.02.03
Strain vs Charge Mediated Magnetoelectric Coupling across the Magnetic Oxide/Ferroelectric Interfaces
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We utilize polarized neutron reflectometry (PNR) in consort with ab initio based density functional theory (DFT) calculations to study magnetoelectric coupling at the interface of a ferroelectric $PbZr_{0.2}Ti_{0.8}O_3$ (PZT)

and magnetic $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) heterostructure grown on a Nb-doped SrTiO3 (001) substrate. Functional device working conditions are mimicked by gating the heterostructure with a Pt top electrode to apply an external electric field, which alters the magnitude and switches the direction of the ferroelectric (FE) polarization, across the PZT layer. PNR results show that the gated PZT/LSMO exhibits interfacial magnetic phase modulation attributed to ferromagnetic (FM) to A-antiferromagnetic (A-AF) phase transitions resulting from whole accumulation. When the net FE polarization points towards the interface (positive), the interface doesn't undergo a magnetic phase transition and retains its global FM ordered state. In addition to changes in the interfacial magnetic ordering, the global magnetization of LSMO increases while switching the polarization from positive to negative and decreases vice versa. DFT calculations indicate that this enhanced magnetization also correlates with an out of plane tensile strain, whereas the suppressed magnetization for positive polarization is attributed to out of plane compressive strain. These calculations also show the coexistence of FM and A-AF phases at zero out of plane strain. Charge modulations throughout the LSMO layer appear to be unaffected by strain, suggesting that these charge mediated effects do not significantly change the global magnetization. Our PNR results and DFT calculations are in consort to verify that the interfacial magnetic modulations are due to co-action of strain and charge mediated effects with the strain and charge effects dominant at different length scale.

B03.02.05
Magnetoelectric Coupling and Magnetic Structure of $RbFe(SO_4)_2$
Junjie Yang; New Jersey Institute of Technology, United States

Multiferroics that simultaneously exhibit ferroelectric and magnetic orders have attracted much attention due to their intriguing physics, such as the nature of the competing magnetic interactions and their coupling to the lattice degree of freedom. Recently, we synthesized single crystals of a new multiferroic material $RbFe(SO_4)_2$ (RFSO). RFSO exhibits an antiferromagnetic transition near 4 K which is associate with the onset of multiferroelectrcity. The electric polarization as a function of magnetic field suggests a strong magnetoelecric (ME) coupling effect in RFSO below 4 K. We also study the magnetic structures of RFSO by neutron scattering technique. In this work, we will discuss the ME coupling effect, the phase diagram and magnetic structures of RFSO single crystal.

B03.02.06
Model for Multiferroic $(NH_4)_2FeCl_5(H_2O)$*
Randy Fishman[1], Jaime Fernandez-Baca[1], Wei Tian[1] and Jan Musfeldt[2]; [1]Oak Ridge National Laboratory, United States; [2]The University of Tennessee, Knoxville, United States

The multiferroic behavior of any material sensitively depends on the microscopic interactions between the spins. We evaluate the magnetic interactions in the multiferroic erythrodsiderite $(NH_4)_2FeCl_5(H_2O)$ by comparing inelastic neutron scattering spectra of a single crystal sample with a simple Heisenberg model containing five exchange interactions and an easy-plane anisotropy. The cycloidal spin state in every *bc* plane is produced by two competing exchange interactions. Using the observed wavevector of this cycloidal spin state as a constraint, excellent agreement is found between the observed and predicted spectra. The exchange and anisotropy parameters also provide excellent agreement with inelastic neutron-scattering spectra in the high-field spin-flop phase. The resulting exchange and anisotropy parameters are compared with the predictions of first-principle calculations.
*Work supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division

SESSION B04.01: Thermal Properties and Phonons

B04.01.01*
Negative Thermal Expansion and Entropic Elasticity in ScF_3 Type Empty Perovskites
Igor Zaliznyak[1], David Wendt[2], Emil Bozin[1], Joerg C. Neuefeind[3], Katharine Page[3], Brent Fultz[4] and Alexei Tkachenko[1]; [1]Brookhaven National Laboratory, United States; [2]Stanford University, United States; [3]Oak Ridge National Laboratory, United States; [4]California Institute of Technology, United States

While most solids expand when heated, some materials show the opposite behavior: negative thermal expansion (NTE). NTE is common in polymers and biomolecules, where it stems from the entropic elasticity of an ideal, freely-jointed chain. The origin of NTE in solids had been widely believed to be different, with phonon anharmonicity and specific lattice vibrations that preserve geometry of the coordination polyhedra – rigid unit motions (RUMs) – as leading contenders for explaining NTE. Our neutron scattering study of a simple cubic NTE

material, ScF_3, overturns this consensus [1]. We observe that the correlation in the positions of the neighboring fluorine atoms rapidly fades on warming, indicating an uncorrelated thermal motion, which is only constrained by the rigid Sc-F bonds. These experimental findings lead us to a quantitative, quasi-harmonic theory of NTE in terms of entropic elasticity of a Coulomb floppy network crystal, which is applicable to a broad range of open framework solids featuring floppy network architecture [2]. The theory is in remarkable agreement with experimental results in ScF_3, accurately describing NTE, phonon frequencies, entropic compressibility, and structural phase transition governed by entropic stabilization of criticality. We thus find that NTE in a family of insulating ceramics stems from the same simple and intuitive physics of entropic elasticity of an under-constrained floppy network that has long been appreciated in soft matter and polymer science, but broadly missed by the "hard" condensed matter community. Our results reveal the formidable universality of the NTE phenomenon across soft and hard matter [1,2].

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B04.01.02
The Dominance of Pure Phonon Anharmonicity on the Thermal Expansion of NaBr
Brent Fultz[1], Yang Shen[1], Claire N. Saunders[1], Camille Bernal[1], Douglas L. Abernathy[2] and Michael E. Manley[2]; [1]California Institute of Technology, United States; [2]Oak Ridge National Laboratory, United States

Thermal expansion depends on the free energy $F(V,T)$ through its mixed second derivative $\partial^2 F / \partial V \partial T$. The equilibrium volume $V(T)$ optimizes $F = E - TS$ by balancing phonon entropy S and elastic energy E. Usually S increases as a material expands (S increases when phonon frequencies are reduced), and E gives a penalty against expansion. Most predictions of thermal expansion use the quasiharmonic approximation (QHA), which assumes only a volume dependence of the phonon frequencies [1,2]. The QHA neglects pure anharmonicity, where phonon frequencies depend on temperature at a fixed volume. Both thermal expansion and entropy depend on all phonons in the crystal, so measuring phonon dispersions by inelastic neutron scattering (INS) enables new and incisive physical tests. Our recent INS study showed that the QHA gave the wrong sign for the thermal frequency shifts of most phonons in silicon [3], and is therefore physically incorrect. Somewhat unfortunately, the QHA did predict adequately the thermal expansion owing to a surprising cancellation of errors. On the other hand, the experimental thermal expansion of NaBr [4] is four times larger than predicted with the QHA. A single crystal of rocksalt NaBr was measured on ARCS at the SNS with 201 rotations in half-degree increments about its [001] axis. Data reduction included a new iterative correction for the multiphonon background from a two-atom crystal, and gave the 4D scattering functions $S(\boldsymbol{Q},E)$. After using Bragg diffractions to assess nonlinearities from the ARCS detector array, the higher Brillouin zones were folded back into an irreducible wedge in the first zone to obtain spectral intensities of the phonon dispersions. These INS measurements reveal an unqualified failure of the QHA to predict the temperature dependence of phonon frequencies in NaBr, even between 10 and 300 K. The changes in experimental phonon dispersions were in excellent agreement with anharmonic theory, using *ab initio* DFT calculations (VASP with s-TDEP [3,5]). The frequencies of longitudinal-optical (LO) phonon modes of NaBr decrease significantly with temperature owing to the real part of the phonon self-energy from cubic anharmonicity [6]. The thermal broadening in frequency of optical modes was nearly as large as their thermal shifts in average frequency (thermal broadening is beyond the QHA). Computation allowed us to pinpoint the origin of the large cubic anharmonicity as arising from first-nearest-neighbor Na-Br bonds. Finally, we note that the temperature dependence of the elastic constants should also depend on anharmonicity.

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B04.01.03
Paramagnon Drag, Magnetic Structure and Dynamics in Li:MnTe
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MnTe is a semiconductor which undergoes antiferromagnetic ordering below its rather high Néel temperature of 307 K. Interestingly, MnTe presents a strong increase in thermopower at the Néel temperature, first reported reported by Wasscher and Haas[1]. This suggests an attractive route to develop this material class for thermoelectric applications. Harnessing the magnetic degree of freedom in thermoelectric materials is an elegant way to mitigate the balancing act of optimizing the counteracting quantities of electronic conductivity and

thermopower. The presence of excess thermopower above the electronic diffusion value and the presence of a spin-Seebeck effect in the paramagnetic state suggest that local thermal magnetic fluctuations of the magnetization give rise to a spin-Seebeck effect similar to that encountered in ferromagnets. Measurements on lightly Li-doped MnTe indicate that a large thermoelectric figure of merit of ZT=1 is possible at T > 800 K, making Li:MnTe the first viable thermoelectric material based on magnetism driven thermopower [2]. Inelastic neutron scattering, nuclear inelastic scattering, and neutron diffraction reveal the lattice[3] and magnetic structure and dynamics and specifically the characteristic magnetic fluctuation frequency and correlation length for the Mn magnetic moments, which are required inputs for a microscopic model of paramagnon drag in the paramagnetic regime. Suprisingly, the paramagnon lifetime of ~30 fs is temperature independent between 307 and 900 K.

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B04.01.04
Nonlinear Propagating Modes Observed beyond the Phonons in Fluorite-Structured Crystals
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The vibrational energy of crystals is known to propagate in quantized sinusoidal waves called phonons. In the realm of nonlinear dynamics, however, nonlinear propagating waves are also possible in the form of cnoidal waves where wave displacements are concentrated in solitons separated by flatter regions – like a train of ocean waves rolling into shore. Nonlinear traveling waves have unique properties that are important in many disciplines including optical communications, conducting polymers, biology, magnetism, and nuclear physics. Yet, despite the crucial importance of crystal lattice vibrations in fundamental and applied science, nonlinear traveling waves have not been observed in ordinary crystals. In this talk we show that nonlinear traveling waves exist in fluorite-structured thoria, urania, calcium fluoride, and barium fluoride using neutron scattering and first-principles calculations. These nonlinear waves are observed as sharp dispersion curves at temperatures ranging from 5 K up to 1200 K, extend to frequencies 30-40% higher than the maximum phonon frequency, and travel at group velocities comparable to or higher than the fastest phonon. Given that these nonlinear modes are still observed at 5 K, our measurements imply that the quantum zero-point motion contains propagating nonlinear modes, or entangled phonons. Prior measurements at reactor-based sources did not probe the high energies where these modes are found because relatively few epithermal neutrons are produced at a reactor source. Our measurements were made possible by the abundant epithermal neutrons available at a spallation neutron source. The existence of these waves in three-dimensional crystals may have ramifications for a wide range of properties.

B04.01.05
Vibrational Entropy of Glass Transitions in Metallic and Molecular Glasses
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When a glass (an amorphous solid) is heated, it softens before crystallization. This soft amorphous phase is a viscous liquid that is deeply undercooled below its usual melting temperature. Significant heat is adsorbed in this “glass transition”, raising the entropy of the material. Different theories, based on indirect experimental measurements, have attributed varying amounts of this entropy (of the glass transition) to changes in vibrational entropy and changes in configurational entropy [1]. For example, the early version of the "potential energy landscape" theory of the glass transition attributes all change in the heat capacity to configurational entropy and does not consider vibrational entropy [2]. The controversy has continued for decades. Our group recently approached this problem directly. Using the high flux and efficiency of ARCS, a direct geometry neutron spectrometer, we measured the vibrational density of

states of a metallic glass as it was heated through its glass transition. This was not possible previously owing to the short times available before crystallization. Data were acquired in event mode, allowing it to be re-binned for analysis over multiple ranges of temperature while preserving statistical accuracy. What we reported in our Nature Physics paper in 2017 [3] was that at most 5% of the entropy of the glass transition originated from vibrational entropy. (We measured the total entropy by calorimetry, and we extracted vibrational entropy from the vibrational density-of-states (DOS) by conventional methods.) The vibrational DOS curves were remarkably similar for the glass, liquid, and crystal phases of Cu-Zr, and the differences for Cu-Zr-Al were also not large.

Very recently, we performed similar inelastic neutron scattering measurements during the heating of two new metallic glasses, $Pt_{57}Cu_{23}P_{20}$ and $Pt_{60}Cu_{20}P_{20}$. These are especially fragile, meaning that they quickly become fluid above the temperature of their glass transitions. Their vibrational spectra are therefore expected to change more strongly at the glass transition than Cu-Zr. In addition, we will report results on the change in the vibrational spectrum of deuterated ortho-terphenyl (1,2-diphenylbenzene, $C_{18}H_{14}$) at the glass transition. Ortho-terphenyl is one of the most fragile glasses because its shear viscosity deviates so strongly from Arrhenius behavior [4]. Analysis of these data is still underway, but we can say that the vibrational DOS of the crystalline forms of these materials is quite different from the amorphous, unlike the case for Cu-Zr. A more complete picture will be presented at the meeting.

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B04.01.07
Magnon-Phonon Interactions in Antiferromagnetic Oxides

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Antiferromagnetic (AFM) materials attract much interests due to their vanishing total magnetization, which allows robustness again disturbance and possible long mean-free-path for applications in spintronics such as magnetoelectric random access memory. Additionally, AFM materials are good candidates for controlling thermal transport via magnetism through external stimuli. In the current work, temperature and field dependent inelastic neutron scattering experiments were performed to investigate the magnon-phonon interactions in nickel (II) oxide and chromium (III) oxide. First principles calculations were performed on antiferromagnetic, non-magnetic, and pseudo-paramagnetic structures to understand the magnon-phonon interactions. The interactions between these excitons are found to be complicated and might have important implications on both the physical properties of phonon lattice dynamics, spin wave, and spin dynamics.

SESSION B04.02: Magnetism in Low-Dimensional Systems

B04.02.01
Signatures of Coupling between Spin Waves and Dirac Fermions in $YbMnBi_2$

Aashish Sapkota[1], Igor Zaliznyak[1], John Tranquada[1], Laura Classen[1,2], Cedomir Petrovic[1], Aifeng Wang[3], Matthew Stone[4], Andrei T. Savici[4], Ovidiu Garlea[4] and Masaaki Matsuda[4]; [1]Brookhaven National Laboratory, United States; [2]University of Minnesota, United States; [3]Chongqin University, China; [4]Oak Ridge National Laboratory, United States

In Dirac materials, coupling of Dirac charge carriers with magnetism can lead to novel phenomena with potential for technological applications [1, 2]. From this perspective, 112 ternary pnictogens $(A,R)MnX_2$ (A=Ca,Sr; R=Yb,Eu; X=Bi,Sb) represent an interesting family of Dirac materials, where both the magnetism and Dirac electrons coexist, thereby providing an opportunity to study the coupling between Mn spins and Dirac electrons in Bi layer [2]. Previous studies of spin excitations in $(Sr,Ca)MnBi_2$ using inelastic neutron scattering (INS) have found no indication of such a coupling because the anomalous broadening found in itinerant magnets was absent [2]. In contrast, our recent INS measurements of spin waves on $YbMnBi_2$ found a small and q-independent broadening in the spin waves, which is consistent with the spin-Dirac fermion coupling. Theoretical calculations show that the effect of the coupling on spin excitations is suppressed by a vanishing carrier density of states at the Dirac point. Nevertheless, the obtained non-negligible coupling constant is still relevant for charge transport by carriers close to the Dirac point.

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B04.02.02

Determination of the Magnetic Order in the $EuIn_2As_2$, an Axion Insulator Candidate

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$EuIn_2As_2$ is a Zintl compound recently reported as a possible first example of axion insulator with antiferromagnetic (AF) longrange order and characteristic colossal negative magnetoresistance. It thus represents a unique platform to investigate the physics of axion insulators and, in particular, to focus on the interplay between the AF order and the topologically protected features of the electronic band structure. Here, we present results from single-crystal magnetic diffraction experiments. Surprisingly, our results reveal the successive stabilization of two different sets of magnetic Bragg reflections indexed with the propagation vectors k_1=(0,0,0.31) and k_2=(0,0,0) below T_{N1}=17 and T_{N2} =15 K, respectively, despite the chemical unit cell containing only a single Eu site. The two magnetic structures are believed to coexist at $T \leq T_{N2}$, and were individually determined from refinement analyses. We will describe both magnetic structures and discuss the influence of our results upon the current understanding of the material's topological features.

B04.02.04

Spin Waves in the Antiferromagnetic Topological Insulator $MnBi_2Te_4$ and $MnSb_2Te_4$

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$MnBi_2Te_4$ is proposed to be the first antiferromagnetic (AF) topological insulator (TI). The natural intergrowth of magnetic and TI layers, and the ground state tunability via a magnetic field provide a unique platform for studying the interplay between magnetism and topological electronic states, which give rise to the quantum anomalous Hall effect and axion electrodynamics. Here we present results from our inelastic neutron scattering (INS) study on $MnBi_2Te_4$ single crystals, where we determined the strength of the magnetic interactions and single-ion anisotropy in the AF state (T_N = 24 K). By comparing our INS data to the dynamic spin susceptibility calculated using a linear-response density functional theory, we find that magnetic interactions up to the fourth nearest-neighbor of Mn are necessary to understand the observed spin wave dispersion. We also present preliminary results of the spin waves in $MnSb_2Te_4$ (T_N = 19 K), which, in addition to the single branch as oberved in $MnBi_2Te_4$, contain another high energy branch due to the presence of an additional magnetic sublattice formed by antisite exchange between Mn and Sb sites. This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. DE-AC02-07CH11358. This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

B04.02.05

Short-Range Magnetic Correlations in the Disordered Ferromagnetic Alloy Ni-V Close to the Quantum Critical Point

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We show small angle neutron scattering (SANS) results of a binary alloy Ni-V that give new insight in the inhomogeneous destruction of a ferromagnet close to a quantum critical point. The ferromagnetic (FM) order of $Ni_{1-x}V_x$ vanishes towards a paramagnetic phase by sufficient substitution of Ni by V. The critical temperature T_c reaches zero towards x_c=0.116 indicating a quantum critical point. Previous magnetization and μSR data noticed magnetic inhomogeneities in Ni-V and in particular found signatures of dynamic magnetic clusters close to x_c, on the paramagnetic side as well as on the FM side [1]. We present new major results of a small angle neutron scattering (SANS) study [2] of polycrystalline Ni-V samples collecting data at NG7SANS at NCNR, NIST and GPSANS at HFIR, ORNL. In Ni-V samples with low T_c<50K we find magnetic short-range correlations in the nm-scale that remain at low temperatures far below T_c in the long-range ordered phase [2]. The remaining fraction of these short-range clusters grows towards x_c and agrees well with the cluster fraction estimate from the magnetization and μSR data [1].

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B04.02.06
Mesoscale Magnetic Structure of Spinel Ferrimagnets
Lazar Kish[1], Alexander Thaler[2], Minseong Lee[3], Matthew Frith[4], Dalmau Reig-i-Plessis[5], Alexander V. Zakrzewski[1], Vivian Zapf[3], Adam Aczel[2], Lisa DeBeer-Schemitt[2] and Gregory MacDougall[1]; [1]University of Illinois at Urbana-Champaign, United States; [2]Oak Ridge National Laboratory, United States; [3]Los Alamos National Laboratory, United States; [4]Argonne National Laboratory, United States; [5]University of British Columbia, Canada

The ferrimagnetic spinels Mn3O4 and MnV2O4 are known for their anomalous magnetoresponsive behavior, including strong magnetoelastic and magnetodielectric coupings. When placed under mechanical stress, these materials show a real-space separation of their volumes into hundred nanometer stripe-like regions of alternating magnetization. In MnV2O4, this domain structure is also accompanied by a hitherto undiscovered superstructure modulation on a shorter lengthscale. I will show small angle neutron scattering data associating these features with known first order magnetic transitions in these materials, and their control via applied magnetic field. I will then draw a direct connection to bulk magnetic measurements, and demonstrate how the stripe domains can lead to anomalous magnetization behaviors.

B04.02.07
Giant Electron-Phonon Coupling of the Breathing Plane Oxygen Phonons in the Dynamic Stripe Phase of La1.67Sr0.33NiO4
Adrian Merritt[1], Dmitry Reznik[1,1], Andrew D. Christianson[2], Arnab Banerjee[2,3], Gu Genda[4] and Andrey Mishchenko[5,6]; [1]University of Colorado, United States; [2]Oak Ridge National Laboratory, United States; [3]Purdue University, United States; [4]Brookhaven National Laboratory, United States; [5]RIKEN Center for Emergent Matter Science, Japan; [6]National Research Center "Kurchatov Institute", Russian Federation

Some of us recently characterized the spectrum of dynamic charge stripes that appears in a 1.67Sr0.33NiO4 (LSNO) above charge-ordering transition temperature of 240K. Here we used inelastic neutron scattering to search for phonon anomalies in the same compound. Most phonons are remarkably insensitive to the transition from static to dynamic stripes, but Ni-O bond-stretching modes that modulate the volume around Ni appear to be an exception. These phonons show giant renormalization on entering the dynamic charge stripe phase with the largest effects observed for the zone boundary half-breathing and breathing modes. The latter undergoes a dramatic collapse, which indicates that dynamic stripe phase hosts small polarons based on the breathing distortion of the NiO6 octahedra. Thus the dynamic stripe phase of LSNO is characterized by coexistence of large polarons in the form of dynamic stripes with small polarons of the breathing type. We argue that formation of small polarons sets the nickelates apart from cuprates where such polarons do not form and point out remarkable similarities between the CMR manganites and stripe-ordered nickelates.

B04.02.08
Quasi-Two-Dimensional Magnetism and Unusual Intermediate Spin State of Tetrahedral Co^{4+} in Ba_2CoO_4
Qiang Zhang[1,2], Guixin Cao[1], Feng Ye[2], Huibo Cao[2], Songxue Chi[2], Masaaki Matsuda[2], William A. Shelton[1], Stephen Nagler[2], Alan Tennant[2], Ward Plummer[1], R. Jin[1] and Jiandi Zhang[1]; [1]Louisiana State University, United States; [2]Oak Ridge National Laboratory, United States

Quasi-two-dimensional (2D) magnetism exists in bulk magnetic materials when the dominant magnetic interactions are intra-planar, which is commonly ascribed to intrinsically layered crystalline structures diminishing the inter-planar coupling through spacing effects. Here, we demonstrate that the material Ba_2CoO_4 exhibits quasi 2D magnetism by combining neutron scattering and linear spin waves theory studies, although the system lacks a clear 2D layered stacking structure and displays comparable nearest-neighbor Co-Co distances. Instead, the reduced quasi 2D magnetism as revealed from the anisotropic spin wave dispersions and magnetic exchange constants is ascribed to a very weak magnetic coupling between two inequivalent quasi-2D Co layers and interpreted

in terms of a frustrated network of super-superexchange pathways Co-O--O-Co where the overlap of the O 2*p*-orbital tails provides the long-range exchange mechanism. Furthermore, the ordered moment, relatively large spin gap and spin-lattice coupling may indicate a very rare intermediate spin state of tetrahedral Co^{4+} as the ground state in Ba_2CoO_4. Our study might reshape the fundamental understanding on the quasi-2D magnetism and provide a new insight on the interplay between coordinate polyhedron, spin exchange interaction, and spin states in Cobaltites.

SESSION B04.03: Skyrmions and Unconventional Magnets

B04.03.01*
Helimagnetism and Chiral Domain Walls in Hexagonal Magnets

John F. DiTusa[1], Sunil K. Karna[1], Madalynn Marshall[1], W. Xie[1], Lisa DeBeer-Schemitt[2], David P. Young[1], Ilya Vekhter[1], William A. Shelton[1], Andras Kovacs[3], Jessica K. Hebert[4], W. A. Phelan[5], Yan Wu[2], Huibo Cao[2] and Damien Tristant[1]; [1]Louisiana State University, United States; [2]Oak Ridge National Laboratory, United States; [3]Forschungszentrum Jülich, Germany; [4]Los Alamos National Laboratory, United States; [5]Johns Hopkins University, United States

Magnetism in non-centrosymmetric (NCS) and chiral structured materials is interesting, in part, because of the importance of an antisymmetric interaction caused by spin-orbit coupling known as the Dzyaloshinskii-Moriya interaction (DMI). The magnetic structures that form in these compounds are largely determined by the exchange interaction along with the DMI and the crystalline anisotropy which is governed by the crystal symmetry. In bulk crystalline materials the competition between these interactions is the cause of long period helimagnetism and have been shown to be key to the formation of skyrmion, hedgehog, and magnetic soliton lattices. We have explored how the balance of these interactions determines the magnetic structures and related behaviors of two hexagonal structured magnets, both NCS with one chiral ($Mn_{1/3}NbS_2$) and one achiral (ScFeGe). We find that these properties depend strongly on the (a)chiral character of the crystal structure. In $Mn_{1/3}NbS_2$, which is formed by intercalating Mn between the layers of the van der Waals compound NbS_2, we observe a somewhat disordered, nearly ferromagnetic state with a magnetization and susceptibility that are sensitive to the application of small fields. Small angle neutron scattering and Lorentz Force Transmission Electron Microscopy measurements confirm these conclusions and reveal chiral domain walls that change character with thickness. For achiral ScFeGe, we find a helimagnetic phase with a period that closely matches a conspicuous nesting of Fermi surface sheets and discover a higher entropy, glass-like, magnetic state at high fields.

B04.03.02
Controlling Long-Range Skyrmion Lattices Using Field and Temperature in Fe/Gd Multilayers

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Ordered magnetic skyrmion lattices presents a lush playground of new and interesting physics to explore. This opportunity is provided, in part, due to the topological nature of the skyrmion. Currently, a significant effort is being made to realize skyrmion-driven devices. These efforts are focused on designing and developing materials that can support skyrmions under ambient conditions. We have recently fabricated thin-films of amorphous Fe and Gd multilayers that support skyrmions and skyrmion lattices at room temperature and zero applied magnetic field. These skyrmions are stabilized by dipolar interactions, rather than the Dzyaloshinskii–Moriya interaction (DMI). By varying the film thickness and alloy composition we can alter the balance of the dipole interactions relative to the exchange and anisotropy we control the skyrmion size, pitch, and stability. Using small angle neutron scattering (SANS), we demonstrated that once formed these dipole skyrmions are stable over a large field and temperature range (including positive/negative/zero magnetic field and temperatures between 10K and 325 K, in a single film). Interestingly, we observe temperature and field dependent changes in the scattering vector (Q) for peak scattering related to the skyrmion lattice spacing. We observed two effects while changing the magnetic field; i). ramping the field results in a decrease in Q suggesting an increased skyrmion

lattice, and ii). when applying an field in the opposite direction to (i), to that used to establish the skyrmion lattice we observe an increase Q before leaving the lattices stability window. The origin of this change in scattering vector has led us to identify a key requirement necessary for the range of stability that we have observed in these amorphous thin films.
Work at UCSD supported by DOE award No. DE-SC0003678. Neutron work was done at HFIR at Oak Ridge National Laboratory supported by DOE Basic Energy Science and NCNR at National Institute of Standards and Technology supported by DOC.
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B04.03.03
Hysteretic Evidence of a Topological Barrier to Skyrmion Lattice Formation in MnSi

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Understanding the complex dynamics of skyrmion formation and destruction is key to developing new technologies which make use of them. Here we report the observation of a hysteresis effect associated with forming and destroying the skyrmion lattice (SkL) in the chiral magnet MnSi using small angle neutron scattering (SANS). This effect is very small when compared to the applied field of the cryomagnet (~ 2 mT vs 200 mT), but is observable and reproducible by the added precision of a custom built solenoid supplementing the cryomagnet. This hysteresis effect is due to the intrinsic topological energy barrier associated with forming the SkL from a non-topological phase. We have further modeled this phase transition with micromagnetic simulations, revealing that it is energetically favorable for the SkL to form progressively in domains of size consistent with sample inhomogeneities.

B04.03.04
Non-Sinusoidal Helical Magnetic Structure in Chiral Helimagnet $Mn_{1/3}NbS_2$
Sunil K. Karna[1], Madalynn Marshall[1], W. Xie[1], Lisa DeBeer-Schemitt[2], David Young[1], Michalis Charilaou[3], Andras Kovacs[4] and John F. DiTusa[1]; [1]Louisiana State University, United States; [2]Oak Ridge National Laboratory, United States; [3]University of Louisiana at Lafayette, United States; [4]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, Germany

We have investigated the magnetic properties of $Mn_{1/3}NbS_2$ formed by intercalating Mn between the layers of hexagonal NbS_2 resulting in a chiral structured magnet. The *ac*- and *dc*-magnetic susceptibility and magnetization, Small-angle Neutron Scattering (SANS), and Lorentz Transmission Electron Microscopy (LTEM) imaging are explored and compared to calculations and micromagnetic simulations. The *ac* susceptibility displays temperature, field, and frequency dependencies which define a complex phase diagram below the critical temperature for magnetic ordering, T_C = 45 K. The magnetic structure was investigated via SANS reveals a streak of magnetic scattering along the *c*-axis near $Q = 0$ appearing below T_C, demonstrating a disordered ferromagnetic (FM) or helical spin ordering. The width of this streak is reduced and becomes more intense near T_C and is gradually suppressed by the application of H along the beam. Micromagnetic simulations of thin lamella are in agreement with LTEM images of $Mn_{1/3}NbS_2$ where extended FM regions result from shape anisotropy in thin samples that are separated by chiral domain walls. All of these measurements display behavior strikingly different from isostructural $Cr_{1/3}NbS_2$ that results from a reduced Dzyaloshinskii-Moriya interaction in $Mn_{1/3}NbS_2$.

B04.03.05
Crystallographic and Magnetic Structure of Pr_2PdSi_3—A Single Crystal Neutron Diffraction Study
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The intermetallic compound series R_2PdSi_3 (R = rare earth metal) exhibits some interesting magnetic properties like giant magnetoresistance effect [2], strong anisotropy in the electronic properties [1] and a generic field induced phase [3]. The magnetic structures are quite complex with large magnetic unit cells due to the delicate interplay between competing crystal electric field effect and magnetic exchange interaction [4] and the addition of geometric frustration. Recently, a Skyrmion lattice has been identified in Gd_2PdSi_3 [5]. This result has been published in a renowned journal and led to a renewed interest in the magnetic properties of this series [6-8]. Complicating the analysis of the magnetic and electronic properties is the fact that the Pd/Si layers obey site occupation rules of its ions and the stacking of the layers yields a crystallographic superstructure [9]. In the R_2PdSi_3 with heavy rare earth ions (R = Gd, Tb, Dy, Ho, Er, Tm) the connection between the crystallographic superstructure and the magnetic

structure has been studied extensively [3]. Summarizing, the magnetic structures are independent of the crystallographic superstructure when the propagation vector lies exclusively in the hexagonal plane (R = Gd, Ho, Er). When the propagation vector contains a non-zero ***c***-component the crystallographic superstructure imposes a modulation of either the magnetic moment value or the in-plane easy axis. In the latter case this leads to a canted antiferromagnetic structure. Recently, the investigations on R_2PdSi_3 have been extended to the light rare earths for instance the Nd_2PdSi_3 where a small antiferromagnetic phase coexists with the dominant ferromagnetic interactions. In our contribution we present a detailed neutron diffraction study on a Pr_2PdSi_3 single crystals [10] using the WAND^2 diffractometer at HFIR. Our study will show that in this compound the crystallographic superstructure is similar to the one observed before, but significantly simpler, leading to only two crystallographic domains instead of six. The compound orders antiferromagnetically at T_N = 2.17K magnetic with the magnetic moments aligned along the c-axis. The magnetic propagation vector is extremely small (1/20, 1/20, 0) without the observation of higher order reflections. Both findings are indication that the ground state of the non-Kramers Pr-ion is non-magnetic and magnetic order is result of perturbation through the crystallographic superstructure in this compound.

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B04.03.06
Spin Structures and Dynamics in Metallic Antiferromagnets
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Recent demonstrations have raised intriguing possibilities of manipulating the Neel vector of antiferromagnets using non-spin-polarized currents, coupling across interfaces, and/or optical excitations. A key feature of these materials is that they should exhibit antiferromagnetic ordering where the Neel vector is degenerate--for example it points along the a or b direction in a tetragonal crystal system. I will discuss our work on the synthesis and characterization of metallic antiferromagnets with degenerate Neel vectors. Until recently, these materials were unheralded and had sparse magnetic structure determinations, especially on single crystals. We present the hexagonal material Cu0.82Mn1.18As, an antiferromagnet with triangular spin arrangment. We also will examine the magnon spectrum and anisotropy of the trilayer antiferromagnet Fe2As. The spin structures and energy scales are not intuitive in this class of materials, and more phases remain to be fully understood.

SESSION B04.04: Iron Pnictides and Related Materials

B04.04.01*
Behaviors of Iron Chalcogenide Spin Ladder BaFe2X3 (X=Se,S) under Pressure
Shan Wu[1,2], Thomas Smart[2], Junjie Yin[3], Craig L. Bll[4], Nicholas P. Funnell[4], Thomas R. Forrest[5], Gediminas Simutis[6], Rustem Khasanov[6], Arani Acharya[2], Meng Wang[3], Benjamin Frandsen[7], Raymond Jeanloz[2] and Robert Birgeneau[2,1]; [1]Lawrence Berkeley National Laboratory, United States; [2]University of California, Berkeley, United States; [3]Sun Yat-Sen University, China; [4]ISIS Neutron and Muon facility, United Kingdom; [5]Diamond Light Source, United Kingdom; [6]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Switzerland; [7]Brigham Young University, United States

In correlated electron systems, electronic phases and phase transitions can be accessed by a variety of tuning parameters including chemical doping and pressure. Relevant phases and phase transitions include metal-insulator transitions, charge density wave order, structural transitions driven by nematic order, anti-ferromagnetism, and superconductivity. In most of the iron- and copper-based superconductors, the superconducting (SC) phase appears when the long range ordered magnetic phase is suppressed by doping carriers, with the majority of them studied to-date exhibiting a two-dimensional square lattice motif. The recent finding of a pressure-induced SC phase (Pc ~ 10 GPa, Tc ~ 24 K) in the iron chalcogenide spin ladder system BaFe2X3 (X=Se,S) has provided a new venue for studying the connection between magnetism and superconductivity without introducing disorder by chemical doping. However, until recently the combination of high pressures and low temperatures has limited the probes of pressure-temperature (P-T) phase diagrams to mainly transport measurements. Elucidating the magnetic and structural properties

requires scattering experiments under pressure, especially neutron scattering. Although in theory neutron diffraction can directly determine the magnetic and crystal structures across the P-T phase diagram, the associated experimental challenges make the tracking of the magnetic transition temperature T_N versus pressure difficult. This can be compensated in part by muon spin relaxation (μSR) measurements, which are sensitive to the magnetic order; and can provide fine control on the size of the steps in pressure and temperature. In this talk, we will present three complementary experimental probes: X-ray powder diffraction (XRD), neutron powder diffraction (NPD) and μSR measurements under pressure in the BaFe2X3; we show how XRD and μSR techniques provide information on the magnetic and structural properties across a large region of the *P-T* phase diagram complementary to that obtained by NPD experiments. We will mainly focus on the BaFe2Se3 ladder system that exhibits a unique block type magnetic order at P = 0. We observe a structural transition at Ps =3.7 GPa as well as a fully ordered robust block-type magnetism up to P = 6.8 GPa. We observe a gradual enhancement of T_N up to Ps followed by a considerable reduction of T_N for P>Ps. These combined measurements provide essential new information on the P-T phase diagram of BaFe2X3, thereby adding new richness to the panoply of iron-based superconductor materials. More generally, we demonstrate that the use of these combined experimental tools provides an effective scientific approach to tackle challenging problems of interest to the neutron community, especially the study of magnetic and structural information under extreme conditions. We also find that there is a compelling need for neutron scattering capabilities combining pressures above 10 GPa and temperatures below 77K.

B04.04.02
Correlated Disorder-to-Order Crossover in the Local Structure of $K_xFe_{2-y}Se_{2-z}S_z$ Superconductor
Robert J. Koch[1], Panagiotis Mangelis[2], Hechang Lei[1], Reinhard Neder[3], Marshall McDonnell[4], Mikhail Feygenson[4], Cedomir Petrovic[3], Alexandros Lappas[2] and Emil Bozin[1]; [1]Brookhaven National Laboratory, United States; [2]IESL FORTH, Greece; [3]University of Erlangen-Nuremberg, Germany; [4]Oak Ridge National Laboratory, United States

A detailed account of the local atomic structure and disorder at 5 K across the phase diagram of the high-temperature superconductor $K_xFe_{2-y}Se_{2-z}S_z$ ($0 \le z \le 2$) is obtained from neutron total scattering and associated atomic pair distribution function (PDF) approaches [1]. Various model-independent and model-dependent aspects of the analysis reveal a high level of structural complexity on the nanometer length scale. Evidence is found for considerable disorder in the c-axis stacking of the $FeSe_{1-x}S_x$ slabs without observable signs of turbostratic character of the disorder. In contrast to the related Fe*Ch* (*Ch* = S, Se)-type superconductors, substantial Fe-vacancies are present in $K_xFe_{2-y}Se_{2-z}S_z$, deemed detrimental for superconductivity when ordered. Our study suggests that the distribution of vacancies significantly modifies the iron-chalcogen bond-length distribution, in agreement with observed evolution of the PDF signal. A crossoverlike transition is observed at a composition of $z \approx 1$, from a correlated disorder state at the selenium end to a more vacancy-ordered (VO) state closer to the sulfur end of the phase diagram. The S-content-dependent measures of the local structure are found to exhibit distinct behavior on either side of this crossover, correlating well with the evolution of the superconducting state to that of a magnetic semiconductor toward the $z \approx 2$ end. The behavior reinforces the idea of the intimate relationship of correlated Fe-vacancy order in the local structure and the emergent electronic properties.

[1] P. Mangelis *et al*., Physical Review B **100**, 094108 (2019)

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B04.04.03
Magnetic Order Arising from Frustrated Interlayer Interactions in Doped $SrCo_2As_2$
John Wilde[1,2], Bing Li[1,2], Andreas Kreyssig[1,2], Benjamin Ueland[1,2], David Vaknin[1], N. S. Sangeetha[1], Yuriy Sizyuk[1,2], Wei Tian[3], Santanu Pakhira[1], Pinaki Das[1,2], Alan I. Goldman[1,2], Peter Orth[1,2], D. C. Johnston[1,2] and R. J. McQueeney[1,2]; [1]Ames Laboratory, United States; [2]Iowa State University of Science and Technology, United States; [3]Oak Ridge National Laboratory, United States

The Fe-based superconductors and their parent compounds offer prime examples of intertwined structural, magnetic, and electronic ground states that can be sensitively tuned by chemical substitution. Some of the observed ground states manifest spin and electronic nematic phases, magnetic frustration, and magnetostructural volume-collapse transitions, and

the interrelationship of these phenomena with superconductivity are central issues in condensed matter physics. With the exception of superconductivity, many of these phenomena extend to the structurally related 122-type tetragonal cobalt arsenides ACo_2As_2 (A = Ba, Ca, Sr, Eu) including magnetic frustration of their square Co layers and As-As hybridization-driven magnetoelastic interactions. Among the tetragonal 122 cobalt arsenides, paramagnetic $SrCo_2As_2$ is particularly interesting because neutron-scattering measurements find antiferromagnetic (AF) stripe-type spin fluctuations similar to those associated with superconducting pairing in the Fe-based superconductors. In addition, ferromagnetic (FM) fluctuations are observed by Nuclear Magnetic Resonance. In principle, tuning the $SrCo_2As_2$ system towards stripe-type AF order through appropriate chemical substitution may realize superconductivity. Here, we present a study of $Sr(Co_{1-x}Ni_x)_2As_2$ [1] and $(Ca_{1-x}Sr_x)Co_2As_2$ [2] single crystals using neutron diffraction and high-energy x-ray diffraction. We find helical-AF order consisting of FM-aligned transition-metal layers stacked AF along **c**. We show that the details of the AF stacking can be described in terms of a one-dimensional Heisenberg model where tuning nearest and next-nearest neighbor interlayer coupling strengths leads to a variety of collinear and noncollinear magnetic ground states. Within the context of metallic quantum materials it is interesting that a local moment model describes well the magnetism within this frustrated itinerant system. Work at the Ames Laboratory was supported by the U.S. Department of Energy (DOE), Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02-07CH11358. A portion of this research used resources at the High Flux Isotope Reactor, a U.S. DOE Office of Science User Facility operated by the Oak Ridge National Laboratory. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the U.S. DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

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B04.04.04
Flat-Band Magnetism and Helical Magnetic Order in Ni-Doped SrCo2As2

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In the AFe2As2 (A = Ca, Sr, Ba) family of iron pnictides, it is well known that the superconducting electron pairing is attributed to antiferromagnetic (AF) spin fluctuations. However, FM spin fluctuations may also be important to electron pairing and were recently observed in Co-substituted compounds by nuclear magnetic resonance and neutron scattering experiments. Furthermore, electronic structure calculations and angle-resolved photoemission spectroscopy (ARPES) experiments indicate that ACo2As2 is in proximity to a FM instability due to the existence of a flat band near the Fermi level, although these materials remain paramagnetic down to 2 K with AF low-energy spin fluctuations. Since chemical substitution can shift the Fermi level relative to the band structure, substitution of Co with Ni will drive the system toward a Van Hove singularity associated with the flat band and efficiently promote the FM instability. Therefore, it is interesting to investigate how AF and FM spin fluctuations evolve in A(Co1−xNix)2As2 and to explore the relevant emergent phenomena. We synthesized a series of Sr(Co1−xNix)2As2 single crystals and obtained a comprehensive phase diagram with respect to field, temperature, and chemical substitution by magnetic susceptibility and magnetization measurements. Our neutron diffraction experiments revealed a helimagnetic order with magnetic moments ferromagnetically aligned in the a b plane and a helimagnetic wave vector of q=(0, 0, 0.56) for x= 0.1. Further Co doping reduces this wave vector and becomes (0,0,0.37) at x = 0.2. Considering both SrCo2As2 and SrNi2As2 are paramagnetic without magnetic order at low temperature, it is surprising that we discovered a helical magnetic order in Sr(Co0.9Ni0.1)2As2. Further analysis of magnetic form factor and angle-resolved photoemission spectroscopy (ARPES) data shows that the helimagnetism is associated with a flat band of dx2-y2 orbital character. On one hand, the helical wave vector with a value nearly equal to (0,0,0.5) can not be explained by the molecular field theory with J1 and J2 model, on the other hand, the existence of a flat band at the Fermi level impose a serious challenge on the estimation of wave vector from Fermi surface nesting picture. We will discuss the possible origin of this helical magnetic order and further evidence of spin fluctuations from inelastic neutron scattering may help understand it.

SESSION B05.01: Topological Materials

B05.01.01*
Quantum Oscillations from Networked Topological Interfaces in a Weyl Semimetal
I-Lin Liu[1,2], Colin Heikes[2], Taner Yildirim[2], Chris Eckberg[1], Tristin Metz[1], Sheng Ran[1,2], William Ratcliff[2], Johnpierre Paglione[1] and Nicholas Butch[2,1]; [1]University of Maryland, United States; [2]National Institute of Standards and Technology, United States
Layered transition metal chalcogenides host many interesting topological electronic phases. $MoTe_2$ has both noncentrosymmetric T_d and centrosymmetric T' structures, associated with a Weyl semimetal and higher-order topology. Pressure tunes the transition temperature between these structures and over a critical pressure range, freezes a mixed T_d-T' matrix at zero-temperature. New quantum oscillations in this critical pressure region indicate a totally different Fermi surface and topology from the topologically nontrivial T_d and T' phases. In this mixed region, we see no evidence for superlattice reflections or missing intensity in elastic neutron scattering measurements. We conclude that a network of topological interfaces gives rise to a new electronic structure.

B05.01.02
Observation of a T_d-1T' Structural Phase Transition at Ambient Pressure in Weyl Semimetal WTe_2
Yu Tao[1], John Schneeloch[1], Adam Aczel[2] and Despina Louca[1]; [1]University of Virginia, United States; [2]Oak Ridge National Laboratory, United States

Layered transition metal dichalcogenides have attract much interest due to their fascinating electronic and mechanic properties. Two of these materials, $MoTe_2$ and WTe_2, are suggested to be Weyl semimetals in the orthorhombic T_d phase, and both show a large non-saturating magnetoresistance. $MoTe_2$ and WTe_2 exist in bulk forms as stacks of strongly in-plane bonded layers with weak van der Waals interlayer interaction and their properties often vary with stacking changes. For example, $MoTe_2$ exhibits a first order structural phase transition at ~260K from a low-temperature orthorhombic T_d phase to a high-temperature monoclinic 1T' phase, with an intermediate pseudo-orthorhombic T_d* phase seen only upon warming. In contrast, the structural properties of WTe_2 have not been studied extensively. Although a pressure-induced transition to a monoclinic 1T' phase has been reported at room temperature, it is long believed that WTe_2 has only the T_d phase at ambient pressure since the material was first structurally characterized many decades ago. However, from the structural phase diagram of $Mo_{1-x}W_xTe_2$, the increase of the transition temperature with W-substitution, measured up to x~0.5, suggests the possibility of a T_d-1T' transition in WTe_2 should be investigated. Neutron scattering experiments at the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL) were conducted on a WTe_2 single crystal. Elastic scans along (2, 0, L) indicate a T_d-1T' structural phase transition in WTe_2 at ~565K. Unlike for $MoTe_2$, the structural transition in WTe_2 proceeds without hysteresis. No intermediate phase is present across the phase boundary, in contrast to the T_d* phase seen in $MoTe_2$. The observation of the 1T' phase in WTe_2 at ambient pressure adds details to the structural behavior of the $Mo_{1-x}W_xTe_2$ family, and gives new insights into re-examination of theories that lack a transition in WTe_2.

B05.01.03
Changes in Interlayer Phonons with Stacking Variation in $Mo_{1-x}W_xTe_2$
John Schneeloch, Yu Tao and Despina Louca; University of Virginia, United States

While it could be very useful to understand how changes in layer stacking arise in quasi-2D materials like $MoTe_2$ where such changes occur with temperature, the small energy differences between these structures makes such a theoretical understanding difficult. $MoTe_2$ provides an especially rich structural system for such study, having three ordered phases (as well as disordered stackings) within a thermal hysteresis loop, all of which can be constructed, to a first approximation, by an A/B sequence of symmetry-equivalent stacking operations. In principle, measuring the interlayer phonons may yield insights into subtle structural differences between stackings and how certain stackings occur. Many low-energy Raman spectroscopy measurements have been done on systems such as MoS_2 and few-layer graphene, but this technique has the limitations that only phonons near the Brillouin zone center and with certain symmetries are observable. We used inelastic neutron scattering to measure interlayer phonons on a single crystal of $Mo_{0.94}W_{0.06}Te_2$ in its T_d, T_d*, and 1T' phases. Measurements were taken at the SPINS instrument at the NIST Center for Neutron Research at the National Institute of Standards and Technology, and at CG4C at the High Flux Beam Reactor at Oak Ridge National Laboratory. Phonon energies were generally consistent with a linear chain model, but softening was seen in T_d* relative to T_d, and on warming in 1T' from 320 to 600 K. Elastic neutron scattering on many $Mo_{1-x}W_xTe_2$ crystals reveal that the spacing between interlayer energy

minima decreases with both W-substitution and warming. Together, these results offer hints into changes in interlayer interactions, and may provide insights into why the transition in $MoTe_2$ proceeds as it does.

B05.01.04
Correlating Magnetic Structure and Magnetotransport in Thin Films of the Weyl Semimetal $Eu_{1-x}Sm_xTiO_3$
Ryan Need[1], Zach Porter[2], Kaveh Ahadi[3], Zhijun Xu[4], Brian J. Kirby[4], Jeffrey W. Lynn[4], Susanne Stemmer[2] and Stephen Wilson[2]; [1]University of Florida, United States; [2]University of California, Santa Barbara, United States; [3]North Carolina State University, United States; [4]National Institute of Standards and Technology, United States

Weyl semimetals (WSMs) are an intriguing class of quantum materials in which the bulk band structure topology generates surface states with linear dispersions near the Fermi energy. In the case of magnetic WSMs, an internal magnetic field breaks time reversal symmetry and results in electronic properties that are strongly dependent on the magnetic structure. In this work, we have used a combination of neutron diffraction and reflectometry to quantify the magnetic structure of thin $Eu_{1-x}Sm_xTiO_3$ films in order to better understand recent magnetotransport results suggesting that this material is a WSM and that Sm doping can drive the Fermi level across the Weyl node. Specifically, we report on the evolution of the average and depth-dependent magnetic order in thin film samples of biaxially strained and electron-doped $EuTiO_3$ for samples across a doping range <0.1 to 7.8 $\times 10^{20}$ cm^{-3}. Under an applied in-plane field, the G-type antiferromagnetic ground state undergoes a continuous phase transition to in-plane field-polarized ferromagnetism. The critical field for ferromagnetism decreases with itinerant carriers, yet the field evolution is qualitatively similar across the doping range. Unexpectedly, we observe interfacial ferromagnetism with saturated Eu moments at low fields that preceeds ferromagnetic saturation throughout the bulk of the film. We bring these results together to paint a complete picture of the materials magnetic structure evolution with doping and field, and discuss its connections to the unusual magnetotransport that has been observed, including anisotropic magnetoresistance and the topological Hall effect.

B05.01.05
Giant Neutron Response in Topological Nodal Semimetals and Topological Superconductors
Mingda Li; Massachusetts Institute of Technology, United States

The experimental determination of a material's topological properties is a complicated task. Conventionally, this task is fulfilled by angular-resolved photoemission spectroscopy (ARPES). However, a few limitations exist, such as limited materials type, high technical barrier, and restricted sample environment. In this talk, we discuss how neutron scattering may be applied to study topological nodal metals and topological superconductors. We will present a new neutron dynamic structure factor formula for a generic topological nodal semimetal based on quantum many-body theoretical calculations. We show that neutron scattering is actually a suitable technique to directly probe the topological features in topological nodal metals. For Weyl semimetals in particular, we show that locations of Weyl nodes within the Brillouin zone, the Fermi velocities of Weyl fermions, which are conventionally accessible through ARPES, and the signatures of the Adler-Bell-Jackiw chiral anomaly, which is inaccessible by ARPES, can all leave hallmark signatures in neutron spectra. These effects remain valid at finite temperature and realistic materials. In parallel, we also introduce how the Majorana bound states in a topological superconductor can be profiled using neutron scattering techniques. Our work offers a neutron-based avenue to probe bulk topological materials, with the capabilities to study a broader materials type with improved versatility, such as to study topological phase transitions.

B05.01.06
Ideal Imperfection for Tuning Magnetic Ground States of van der Waals Quantum Materials
Yaohua Liu, Jiaqiang Yan, Xiaoping Wang, Bryan Chakoumakos and Yan Wu; Oak Ridge National Laboratory, United States

Magnetic van der Waals (vdW) quantum materials provide a fertile playground to pursuit novel device concepts, such as Lego heterostructures and Moiré heterostructures. At the same time, when magnetic vdW materials are decorated with nontrivial topological band structures, massive Dirac gaps can form and more exotic quantum states of matter may be realized, such as the axion insulator and Chern insulator phases that can give rise to dissipationless electronics or topological magnetoelectric effects at elevated temperatures. To utilize a magnetic vdW material as building blocks for spintronics, it is often of great importance to achieve a certain nonvolatile magnetic ordering state. Here we demonstrate that structural imperfections can provide a simple route toward this end. Particularly, we show that the interlayer coupling of a vdW material $MnSb_2Te_4$ can be dramatically tuned from the antiferromagnetic to the ferromagnetic state through the unavoidable site intermixing. In $MnSb_2Te_4$, each two-dimensional

(2D) layer block consists of septuple atomic layers and these 2D layer blocks are weakly bound to each other by vdW forces. Magnetometry studies suggest that flux-grown $MnSb_2Te_4$ crystals show either antiferromagnetic-like or ferromagnetic-like behaviors. We have conducted single-crystal neutron diffraction experiments on a series of crystals and the results have been cross-checked at three different single-crystal neutron diffractometers, namely, time-of-flight diffractometers CORELLI and TOPAZ at SNS and a constant-wavelength diffractometer HB-3A at HFIR. There is unambiguous evidence that each crystal shows one of two different magnetic ordering wavevectors, i.e., $\mathbf{k_F}$ = (0,0,0) or $\mathbf{k_{AF}}$ = (0,0,1.5). Chemical structure refinements show that the two different magnetic ground states are correlated with subtle differences in the Mn/Sb site-intermixing. Crystals with more Mn at the Sb site show ferromagnetic interlayer coupling with $\mathbf{k_F}$ = (0,0,0), while those with less Mn ions sitting at the Sb site favors antiferromagnetic interlayer coupling with $\mathbf{k_{AF}}$ = (0,0,1.5). However, in both types of crystals, the magnetic moment on Mn ions at the Sb site is aligned antiparallel to those of Mn ions at the Mn site. We propose a phenomenological model that the sign and the strength of the effective inter-septuple-layer coupling is sensitive to the level of the Mn/Sb site-intermixing. This work shows an unconventional aspect of utilizing structural imperfections in vdW quantum materials, and such an ideal-imperfection approach can be generalized to tune the magnetic ground state of similar vdW compounds, particularly the topological insulator candidate $MnBi_2Te_4$ that is currently under intensive study. This research used resources at the Spallation Neutron Source and High Flux Isotope Reactor, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory, and was partially supported by U.S. DOE, Office of Science, BES, MSED.

B05.01.07
Magnetic Interactions in the 2D Layered van der Waals Semiconductor $CrPS_4$
Stuart Calder[1], Amanda Haglund[2], Yaohua Liu[1], Daniel M. Pajerowski[1], Huibo Cao[1], Travis J. Williams[1], Ovidiu Garlea[1] and David Mandrus[2]; [1]Oak Ridge National Laboratory, United States; [2]University of Tennessee, Knoxville, United States

Materials in which the interactions are confined to two-dimensional (2D) layers offer routes to enhanced quantum behavior and potential functionality in next generation devices. Consequently, there has been recent interest in the class of materials that host isolated 2D layers weakly connected by van der Waals (vdW) bonding. These 2D vdW materials show intriguing behavior in the bulk, including signatures of Skyrmions, Anomolous Hall effect and emergent quasi-particles. The weak vdW bonding means the structure can often be reduced down to the single layer limit. $CrPS_4$ is such a 2D vdW material that is an intrinsic semiconducting magnetic, however has undergone only limited experimental investigations to date. Here we present a series of neutron scattering measurements to uncover the underlying spin behavior. The magnetic structure is determined and a subtle spin reorientaiton identified. Inelastic neutron measurements (INS) provide a highly constrained exchange interaction model Hamiltonian. This is despite the measurements being on a powder since a balance of interaction strengths leads to a sharp separation of observed magnetic excitations due to a region of anomalously low intensity in the measured S(Q, ω). The results reveal the subtle role of competing interactions in 2D vdW materials, which manifest in a non-trivial magnetic transition and a tunable magnetic structure with small applied fields. Our results in the bulk compound provide intriguing insights that can be applied to an understanding of the behavior of reduced layer $CrPS_4$.

SESSION B05.02: Superconductors and Other Materials

B05.02.01
Identifying and Solving Weak Magnetic Phases in $LaFeAs_{1-x}P_xO$ Superconductors with Neutron Powder Diffraction
Ryan S. Stadel[1,2], Stephan Rosenkranz[1], Matthew J. Krogstad[1], Raymond Osborn[1], Dmitry Khalyavin[3], Pascal Manuel[3], Rafael Fernandes[4], Morten Christensen[4] and Omar Chmaissem[1,2]; [1]Argonne National Lab, United States; [2]Northern Illinois University, United States; [3]Rutherford Appleton Laboratory, United Kingdom; [4]University of Minnesota, United States

Neutron diffraction is an invaluable tool for identifying magnetic structures. For materials with strong magnetic moments, especially if large crystals can be grown, solving a new magnetic structure is a straightforward, if often still non-trivial endevour in material sciences. However, for materials with many dynamic phases competing for electrons in narrow regions of composition, magnetic scattering from the prevailing phase can be quite elusive. We present the results of a series of experiments which pushed the limits of some of the highest flux high-resolution

neutron diffraction instruments availble and the methods necessary to work within those limits to identify new magnetic phases. Neutron powder diffraction was performed on $LaFeAs_{1-x}P_xO$ superconductors on POWGEN at the SNS at ORNL as well as WISH at ISIS at RAL. We identified structures on three magnetic phases, two of which were unreported in literature and had magnetic moments less than 0.2 μ_B. By combining neutron diffraction for structural analysis with muon spin resonance on EMU at ISIS at RAL for temperature dependence, we completed a detailed phase diagram including the newly discovered structures.

B05.02.02
Magnetic Structures in the Vicinity of the Pressure-Induced Superconducting Phase in $CeNiC_2$
Depei Zhang[1], Jun Gouchi[2], Feng Ye[1], Takahiro Matsuoka[3], Toru Shigeoka[4], Yoshiya Uwatoko[2] and Masaaki Matsuda[1]; [1]Oak Ridge National Laboratory, United States; [2]The University of Tokyo, Japan; [3]The University of Tennessee, Knoxville, United States; [4]Yamaguchi University, Japan

Recently, the non-centrosymmetric ternary lanthanide nickel carbide, $CeNiC_2$, was reported to show multiple magnetic phase transitions below 20 K[1]. Most importantly, this compound exhibits heavy-fermion superconductivity below 3.5 K under high pressure [2]. However, the magnetic structures of $CeNiC_2$ have not been well studied. In order to understand the superconducting pairing mechanism, it is important to characterize the magnetic structure in the vicinity of the superconducting phase. This talk will focus on the high-pressure neutron diffraction study of the magnetic structures of $CeNiC_2$. An incommensurate antiferromagnetic phase is observed in a wide pressure range from ambient pressure to the pressure where superconducting phase is induced. The magnetic structures identified from both polarized and unpolarized elastic neutron scattering measurements and their connections to the superconductivity will be discussed in detail.

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B05.02.03
Hidden Hydrogen and a Spin-Glass to Superconducting Transition in Quasi-1D KCr_3As_3
Keith M. Taddei[1], Liurukara Sanjeewa[1], Bing-Hua Lei[2], Yuhao Fu[2], Qiang Zheng[1], David Singh[2], Athena Sefat[1] and C. R. Dela Cruz[1]; [1]Oak Ridge National Laboratory, United States; [2]University of Missouri, United States

In the race to find topological materials, superconductivity has found renewed interest as a potential host of Majorana Fermions. However, realizing such states is non-trivial requiring for instance Cooper pairs with finite orbital-momentum or Dirac-like dispersions in the normal state. Recently, a new family of quasi-1D superconductors $A_{1,2}Cr_3As_3$ (A= Alkali metal) was discovered which is interesting in these regards for realizing spin-triplet superconductivity and having Dirac-like crossings near E_F. However, its study has been hampered due to extreme air sensitivity and an inability to charge dope. Here, we report results of diffraction studies and DFT work on KCr_3As_3 which solve both these problems. We show that the reported growth technique inherently intercalates H into the quasi-1D CrAs tubes and that the H acts as an electron donor. Furthermore, we reveal that the reported discrepancy in sample behavior (with some superconducting and others spin-glasses) is actually due to the amount of H. This work suggests a new stoichiometry $KH_{1-x}Cr_3As_3$, which is air stable and provides a charge doping mechanism. This allows for tuning between frustrated magnetism and superconductivity in a quasi-1D material as well as a potential route to reach the predicted Dirac points.

B05.02.04
Ground State Magnetic Structure of Mn3Ge
Jian Rui Soh[1], Fernando de Juan[2], Navid Qureshi[3], Henrik Jacobsen[4], H.-Y. Wang[5], Y.-F. Guo[5] and Andrew Boothroyd[4]; [1]EPFL, Switzerland; [2]Donostia International Physics Center, Spain; [3]Institut Laue-Langevin, France; [4]University of Oxford, United Kingdom; [5]ShanghaiTech University, China

We have used spherical neutron polarimetry to investigate the magnetic structure of the Mn spins in the hexagonal semimetal Mn3Ge, which exhibits a large intrinsic anomalous Hall effect. Our analysis of the polarimetric data finds a strong preference for one of the symmetry-allowed spin structures. We show that weak ferromagnetism is an inevitable consequence of the symmetry of the observed magnetic structure, and that sixth order anisotropy is

needed to select a unique ground state.

B05.02.06
Synthesis and Characterization of Metastable Functional Phases of Germanium
Bianca Haberl, Mary-Ellen Donnelly, Yan Wu, Matthias D. Frontzek, Jamie J. Molaison and Garrett E. Granroth; Oak Ridge National Laboratory, United States

This work here combines *in situ* high pressure diffraction on the WAND^2 beamline of the High Flux Isotope Reactor with inelastic neutron scattering on recovered samples on the ARCS beamline of the Spallation Neutron Source for the study of functional metastable phases of germanium. Such metastable phases of silicon and germanium afford the opportunity of useful functionality different from standard diamond-cubic Si and Ge while allowing for easy integration into existing technology. They could potentially yield an Si or Ge structure with ideal band gap characteristics for solar power conversion, improved thin-film characteristics or – in form of a hydride - even for very high temperature superconductivity. These metastable phases can be synthesized through the application of high pressure. For example, standard Si and Ge transform to a metallic phase with the structure of white tin when compressed to ~11 GPa. Decompression from this metallic phase results in the formation of various metastable phases that are kinetically stable at ambient conditions, have band gap characteristics different from their parent material and could thus be technologically exploited. Here, we characterize the simple tetragonal structure of Ge, the so-called st12-Ge by inelastic neutron scattering. Therefore, st12-Ge is synthesized using double-toroidal diamond anvils in a Paris-Edinburgh press from small pieces of a Ge wafer. The sample is pressurized to above 15 GPa and kept at maximum pressure for several hours to ensure full conversion to the metallic phase. No pressure medium and a very slow decompression rate are used to improve yield of the st12 phase. This synthesis pathway is observed *in situ* on WAND^2 on a representative sample. The 15 GPa applied during synthesis represent thereby the highest pressure applied to a sample at HFIR to date. Subsequently, the phonon density of states of such st12-Ge is determined on the ARCS spectrometer. While many studies have investigated these metastable phases and also st12-Ge by density functional theory, this is the first experimental study of its phonon density of state. This thus yields unique insights into its potential as future semiconductor material.

B05.02.07
Vacancy-Driven Variations in the Phonon Density of States of Fast Neutron Irradiated Nuclear Graphite
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Research studies into the subject of radiation damage and effects in graphite began in the early 1940's during the development of moderated nuclear reactors. Interest in this topic is expanding because of emerging applications associated with fullerenes and carbon nanostructures as well as its long-standing use as a fission moderator. Radiation damage in graphite has been explored via several experimental techniques, such as high-resolution transmission electron microscopy, atomic force microscopy, scanning tunneling microscopy, Raman spectroscopy and x-ray photoelectron spectroscopy. Measurements of lattice excitations offer another mechanism to study radiation damage in graphite. In this work, a series of measurements of the scattering functions of un-irradiated and highly irradiated samples of nuclear graphite were performed at room temperature using the Wide Angular-Range Chopper Spectrometer at the Neutron Spallation Source in Oak Ridge National Laboratory. The graphite samples we examined were exposed to different levels of neutron doses and irradiation temperatures within the core of the High Flux Isotope Reactor[1]. A super-resolution reconstruction technique[2] was used to obtain the phonon densities of states from the measured scattering functions. The phonon densities of states of many defected supercells with a different vacancy and interstitial configurations were calculated using the first-principles direct method. Our measurements show that the scattering functions of the irradiated samples become more diffuse with increasing neutron dose and the induced damage is localized. The calculations predicted very well the variations in the irradiated graphite samples phonon densities of states and indicated that these variations are mainly attributed to the formation of vacancies.

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Acknowledgments: The irradiation of the specimens was performed at the Oak Ridge National Laboratory (ORNL) and sponsored by Tokai Carbon Co., Ltd. (NFE-09-02345) with the U.S. Department of

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B05.02.08
Spin Excitations in Multiferroic Skyrmion Host GaV_4S_8
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In the lacunar spinel GaV_4S_8, the interplay of spin, charge, and orbital degrees of freedom results in a complex phase diagram that includes ferroelectric, orbitally ordered and Néel type skyrmion phases. GaV_4S_8 exhibits a cycloidal state at zero field and a Néel type skyrmion spin structure with the application of field below 12.7 K. To understand the physics driving the formation of these novel phases, we have carried out inelastic neutron scattering measurements on GaV_4S_8 above and below the ordering temperature of 12.7 K. Dispersive spin excitations with a zone boundary energy near 5.7 meV are observed along the [100], and [110] directions within the magnetically ordered phase. Using Heisenberg model with near neighbor exchange couplings and Dzyaloshinskii-Moria (DM) interactions, the excitation spectra are simulated. Simulation shows ferromagnetic inter-tetrahedral couplings with J= -0.76(3) meV along x, y and -0.60(3) meV along z-direction. It is also observed that the DM interactions are around an order of magnitude weaker than the nearest neighbor exchange interactions. A small and finite value of the DM interaction at 2 K provides evidence that the ground state of GaV_4S_8 is a cycloid below the ordering temperature in zero applied field.

Poster Session: Hard Condensed Matter

PB.01.02
Magnetic Field Induced Antiferromagnetic Cone Structure in Multiferroic $BiFeO_3$
Masaaki Matsuda[1], Sachith Dissanayake[2], Tao Hong[1], Yasuko Ozaki[3], Toshimitsu Ito[3], Masashi Tokunaga[4], Xinzhi Liu[5], Maciej Bartkowiak[5] and Oleksandr Prokhnenko[5]; [1]Oak Ridge National Laboratory, United States; [2]Duke University, United States; [3]National Institute of Advanced Industrial Science and Technology, Japan; [4]University of Tokyo, Japan; [5]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

Neutron diffraction measurements were performed under high magnetic fields up to 17 T in a multiferroic $BiFeO_3$, in which an intermediate magnetic (IM) phase has been found between the cycloid and canted antiferromagnetic phases [1]. We clearly found that the incommensurate magnetic peaks, which split perpendicular to the magnetic field in the cycloid phase, rotate by 90 degrees to align parallel to the field in the IM phase. The magnetic structure in the IM phase can be best described by an antiferromagnetic cone (AF-cone) structure. The transition from the cycloid to AF-cone is the first order and the direction of the magnetic wave vector and the easy plane of the cycloidal component are rotated by 90 degrees without changing the cycloidal modulation period, whereas the transition from the AF-cone to canted antiferromagnetic phase is gradual and the cone angle becomes smaller gradually without changing the modulation period. Interestingly, the cycloidal component as well as the cone angle in the IM phase shows a large hysteresis between the field increasing and decreasing processes. This result, combined with the magnetostriction with a large hysteresis previously reported in the IM phase, suggests a strong magnetoelastic coupling.
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PB.01.03
Lessons from $La_{1.67}Sr_{0.33}NiO_4$ on Decoupled Spin Excitations within Charge Stripes
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It is well established that charge and spin stripe orders develop in $La_{1.67}Sr_{0.33}NiO_4$ on cooling. While the spin stripes develop two-dimensional order, there are also spin degrees of freedom on the charge stripes. Evidence of 1D spin correlations from the charge stripes was first provided by the neutron scattering study of Boothroyd *et al*. [1]. We have recently confirmed the 1D character of these excitations and have shown that they become apparent at low temperature when the charge stripes become dominantly Ni-centered [2]. The decoupling of the spins on the charge stripes from the surrounding spins is due to the antiphase character of the spin stripe order, which causes the interaction to be geometrically frustrated. This effect provides an important lesson for stripe order in cuprates such as $La_{1.875}Ba_{0.125}CuO_4$ [3], and how to interpret the observed spin excitations in such systems. In the cuprate case, the spin degrees of freedom on the charge stripes have a large gap that corresponds with the energy scale below which the spin stripe excitations are antiphase. Above that scale, the excitations have a singlet-triplet character with a very short correlation length.
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PB.01.04
Yb Dimers in Perovskite Material $Y_{0.95}Yb_{0.05}AlO_3$
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Yb ions in $YbAlO_3$ tends to form chains where each Yb only couples with its two neighbors along the c-axis. Here we present a study of the Yb dimers in a perovskite material $Y_{0.95}Yb_{0.05}AlO_3$. We used Monte-Carlo calculations to estimate the probability of Yb multimer. Low temperature specific heat demonstrates that dimers dominate the specific heat signal at zero field. Inelastic neutron scattering was used to study the magnetic excitations. The L-modulated stripe-like excitations which appear around 0.21 meV are proved to stem from Yb dimers. The magnetization results show that the magnetic moments of Yb ions are confined in ab-plane with the same magnetic anisotropy and a proximate value of saturation moment with pure $YbAlO_3$.

PB.01.05
Neutron Study on Average and Local Structure in Se-Doped $Ge_2Sb_2Te_5$ Materials
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Phase change material, $Ge_2Sb_2Te_5$ (GST-225), has been used in non-volatile electronic memories found in flash drives. This is because of its rapid reversible phase transition between amorphous and crystalline phases accompanied by a very large change in the electric resistivity and optical reflectivity. In GST-225, the amorphous phase only appears in thin film form because a rapid cooling rate (~10^6K/s) is required to quench the system to the amorphous state. However, by doping with Se as in $Ge_2Sb_2Se_{5x}Te_{5-5x}$ (GSST-225, $0<x<1$), we found that the amorphous phase can be stabilized using liquid nitrogen quenching. Through systematic doping, we observed a crystalline-to-amorphous phase transition at x = 0.9 in liquid nitrogen quenched samples while the as-grown samples remain crystalline across the entire doping range. Measurements of the electric resistivity showed that both the as-grown and liquid nitrogen quenched samples exhibit a metal-to-insulator transition (MITs) around x=0.9 even though the as-grown GSST is crystalline. We investigated the atomic structure of GSST-225 as a function of doping. The Rietveld refinement on the liquid nitrogen quenched samples, x ~0 0.8, indicates coexistence of three phases: a majority GSST-225 hexagonal phase (~70%), a secondary GSST-225 cubic phase (~20%) and a third GSST-124 hexagonal phase (~10%). By x=0.85, a mixture of amorphous and crystalline phases is observed with a distinct pre-peak commonly observed in amorphous systems. By x = 0.9, the liquid nitrogen quenched samples are amorphous. The local atomic structure obtained using the pair distribution function (PDF) analysis on quenched samples shows that in spite of the fact that x = 0.9 is amorphous, short-range correlations are very well preserved. These short range correlation peaks are the same as the ones observed in crystalline x = 0.8, while the medium and long-range features are damped. These results indicate that although globally amorphous, local short range order exits. Measurements of the density of states (DOS) on quenched samples show a valence band feature close to 6 eV on binding energy, which implies the presence of band like features that are persistent even

in the amorphous samples.

PB.01.06
A Comparative Study of Complex Magnetic Structure Determination Using Irreducible Representation Modes and Magnetic Superspace Group

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The complex magnetic structure of a new decorated spin-chain compound $Rb_2Mn_3(MoO_4)_3(OH)_2$ (RbMnMo) has been determined from single crystal neutron diffraction experiments conducted at CORELLI, SNS [1]. We have used a comparative data analysis approach using the irreducible representation (irreps) modes and the magnetic superspace group (MSSG). The compound's crystal structure contains bond-alternating $[Mn_3O_{11}]^{\infty}$ chains along the *b*-axis, formed by isosceles triangles of Mn ions occupying two crystallographically nonequivalent sites (Mn1 site on the base and Mn2 site on the vertex). These chains are only weakly linked to each other by nonmagnetic oxyanions. On cooling, it transitions from a paramagnetic phase into an incommensurate phase below 4.5 K with a magnetic wavevector near $\mathbf{k}_1$ = (0, 0.46, 0). An additional commensurate antiferromagnetically ordered component arises with $\mathbf{k}_2$ = (0, 0, 0), forming a complex magnetic structure below 3.5 K with two different propagation vectors of different stars. On further cooling, the incommensurate wavevector undergoes a lock-in transition below 2.3 K.
For the commensurate component, the irrep modes and the magnetic space group give equivalent magnetic structure models. For the incommensurate structure, the operation that interchanges **k** and **-k** was overlooked in the traditional representation analysis, which splits the Mn1 site into two independent sites, forming a pair of orbits related by the space inversion operation. Therefore, MSSG gives riser to a more robust model. This agrees with recent advancement in the MSSG methodology and software, which shows that MSSG generally introduces either stricter or equivalent restrictions on the incommensurate magnetic structures than the irrep modes alone [2]. The experimental results suggest that the magnetic superspace group is **Pnma.1'(0b0)s0ss** for the single-***k*** incommensurate phase and is **Pn'ma(0b0)00s** for the 2-***k*** magnetic phase. We propose a simplified magnetic structure model taking into account the major ordered contributions, where the commensurate $\mathbf{k}_2$ defines the ordering of the *c*-axis component of Mn1 magnetic moment, while the incommensurate $\mathbf{k}_1$ describes the ordering of the *ab*-plane components of both Mn1 and Mn2 moments into elliptical cycloids.
This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

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PB.01.07
SANS Analysis of the Ferromagnetic Alloy Ni-V with Random Atomic Distribution

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We present a small angle neutron scattering (SANS) analysis of the ferromagnetic alloy $Ni_{1-x}V_x$ which can be driven to a paramagnetic phase by random chemical substitution of Ni by V at x_c=0.116 [1] to find the relevant magnetic correlations at this quantum phase transition. Data of polycrystalline $Ni_{1-x}V_x$ samples with x=0.10 and x=0.11 with low critical temperatures T_c<50K were collected at NG7SANS at NCNR, NIST and GPSANS at HFIR, ORNL. We mainly focus on half and full polarized neutron data [2] with magnetic field perpendicular to the beam to better resolve the small magnetic response from nuclear and other background scattering. In particular, we demonstrate the advantages and limitations of extracting the different magnetic components at different wave vector regimes (within $q=0.06\text{-}1nm^{-1}$) using the angular dependence of spin-flip and non-spin-flip interference cross sections. For both Ni-V samples we find isotropic magnetic short-range correlations that are suppressed in higher fields. In addition, we resolve anisotropic magnetic contributions revealing large-scale magnetic domains below T_c and magnetic defect scattering remaining in high fields. We present possible simple quantitative descriptions and their limitations. These SANS data confirm magnetic correlations at multiple length scales in $Ni_{1-x}V_x$ close to x_c.
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PB.01.08

Magnetic Characterization of Pt/$Tb_3Fe_5O_{12}$ Thin Films by Polarized Neutron Reflectometry

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The insulating ferrimagnets of rare-earth iron garnets (ReIG) have been intensively studied over the past decade due to their strong magneto-electric responses and magneto-optical properties [1]. In this work, Pt/$Tb_3Fe_5O_{12}$ (TbIG) bilayer thin films were grown on (111) single crystalline $Gd_3Ga_5O_{12}$ (GGG) substrates by using the pulsed laser deposition (PLD) technique [2]. The magnetic properties of the Pt(1 nm)/TbIG(27 nm) bilayer were characterized below, above, and near the TbIG compensation temperature ($T_{comp.}$) by polarized neutron reflectometry (PNR) [3]. The neutron reflectivity with different states (spin up (R_+) and spin down (R_-)) was measured as a function of scattering vector Q (=(4psinq)/l).Results have shown that the neutron reflectivity at 8 K exhibits the clear splitting of R_+ and R_-, indicating strong magnetization (saturation magnetization $M_s = 1.1\ \mu_B$) in the Pt/TbIG bilayer. As expected, the magnetization decreases with increasing temperatures. The spin asymmetry (SA = (R_+-R_-)/(R_++R_-)) results are consistent with those obtained by the temperature dependence of the magnetization. The scattering length density (SLD) models were developed to successfully fit the data. Using a four-layer model, two ferromagnetic layers at the interface above ($M_s = 0.05\ \mu_B$) and below ($M_s = 3.75\ \mu_B$) the TbIG layers at 8 K were found, as shown by the magnetic depth profile. This is attributed to the magnetic proximity effect between the TbIG film and the Pt layer and the GGG substrate, respectively. The research was supported by MOST of Taiwan, RGC of HKSAR (PolyU 153027/17P), ANSTO, and University of Wollongong, Australia.

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PB.01.09

Magnetism in Honeycomb Na2Ni2TeO6 with Chiral Layers of Na

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Low dimensional magnetic lattices are being studied recently owing to the possibility of realizing flatbands in the magnon spectrum which can then lead to dissipation-less spin transport and associated magnon Hall effect. One could expect to find a magnon insulator, similar to an electronic topological insulator. In the present work we present a rather less-studied honeycomb magnet $Na_2Ni_2TeO_6$, where Ni^{2+} constitutes the honeycomb lattice. Our samples of $Na_2Ni_2TeO_6$ conform to hexagonal *$P6_3/mcm$* space group with refined lattice parameters, a = 5.2023(1) Å and c = 11.1552(8) Å. The physical properties of the present sample are characterized using magnetic susceptibility upto 1.2 GPa and specific heat in 0 T and 8 T, both of which confirm a phase transition at 28 K. Application of 8 T magnetic field only slightly polarizes the transition. We obtain a Curie-Weiss temperature of -9.7(2) K and effective paramagnetic moment of 2.24(4) m_B/Ni. This matches well with the spin-only moment of Ni^{2+}. We determine the magnetic structure of $Na_2Ni_2TeO_6$ dictated by two propagation vectors – one commensurate and the other, incommensurate. Inelastic neutron scattering experiments reveals a rather flat spin wave excitation at 5 meV. Combining neutron scattering data with density functional theory computations, we arrive at the conclusion that a third in-plane nearest neighbor interaction is essential to understand the magnetism of the honeycomb layers of Ni in $Na_2Ni_2TeO_6$.

PB.01.11

Temperature Dependent Lattice Dynamics in Iridium

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The characterization of simple elemental systems can provide key information to cross-validate first principles modelling and advance our predictive design capabilities. One of these elemental systems, iridium, has received surprisingly little attention experimentally although it is of special interest due to

its large relativistic effects and electron-phonon coupling. In a first step towards a better understanding of the thermodynamic and electronic properties of iridium, we have collected inelastic neutron scattering by a thin polycrystalline sheet of iridium in order to obtain the phonon density-of-states between 10 and 873 K. These data are compared with DFT calculations and provide a deeper understanding of anharmonic effects and the lattice thermodynamic properties. We find that the experimental Grüneisen parameter obtained from the transverse and longitudinal acoustic van Hove singularities are 4.5 and 2.3, respectively, indicate a substantial anharmonicity. Work supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

PB.01.13

Correlated Disorder in Cuprate Superconductors Studied by Neutron Diffuse Scattering

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Nanoscale inhomogeneity is a well-known feature of the cuprate superconductors, but it remains unclear what effect this inhomogeneity has on the physics of these materials. Recent studies of superconducting fluctuations above T_c have revealed a universal inhomogeneity-driven regime in cuprates [1-3] and other unconventional superconductors [4], which may be driven by universal structural distortions [4]. We performed neutron diffuse scattering measurements of several cuprate superconductors using the CORELLI spectrometer at the SNS [5]. These measurements, in combination with complementary X-ray diffuse scattering measurements and the 3D-ΔPDF method [6] for determining real-space structure, reveal short-range correlated structural disorder. We discuss the doping and temperature dependence of these local distortions.

PB.01.16

Phase Transitions in Novel Li-Containing Honeycombs, Li8Cr2(Te/Sb)O12

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Octahedral layers of metal atom separated and charge-compensated by alkali-metal ions have the ideal architecture to be used as electrodes for Li-ion batteries, ionic conductors, and visible light photocatalysts. $Li_8M_2(Te/Sb)_2O_{12}$ (M = transition metal) are relatively new members of this class. Forming honeycomb frameworks, they present interesting magnetic phenomena related to frustrated two-dimensional lattices of spins. In the present work, polycrystalline $Li_8Cr_2(Te/Sb)_2O_{12}$ were synthesized by standard solid-state route. Neutron diffraction experiments were performed at POWGEN, ORNL and $C_{2/m}$ space group was confirmed for both the compounds using Rietveld analysis. The lattice parameters determined are a = 5.141 Å, b = 8.884 Å, c = 5.143 Å, β = 109.5 Å for $Li_8Cr_2Sb_2O_{12}$, and a = 5.128 Å, b = 8.850 Å, c = 5.151 Å, β = 109.8 Å for $Li_8Cr_2Te_2O_{12}$, presenting diminished unit cell sizes compared to that of Li8Co2Te2O12 are a = 5.226 Å, b = 8.892 Å, c = 5.160 Å, β = 110.9 Å. In the case of $Li_8Cr_2Sb_2O_{12}$ a magnetic phase transition is present at 7.4 K as determined from the derivative, dCp/dT. A similar transition is found in $Li_8Co_2Te_2O_{12}$ at 9.5 K. Though broad phase transitions are visible in the bulk measurements, our neutron diffraction data down to 1.7 K do not indicate the presence of long-range ordered magnetism. We will present the details of the structure, mixed occupation of Li and Cr in the lattice and the connection with broad features in magnetic susceptibility. Microscopic understanding of the structure of these honeycombs with Li will be useful in research related to cathodes for batteries.

PB.01.17

Na Diffusion and Phonon Dynamics in Na_3PS_4 and Na_3PSe_4—A Combined Study with Inelastic Neutron Scattering and First-Principles Simulations

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Sodium-based solid-state batteries constitute a promising alternative to current lithium technology, owing to the high abundance of sodium [1]. However, traditional Na-based solid electrolytes (SE), such as β-alumina and so-called NASICON compounds, have so far exhibited only limited ionic conductivities. Encouragingly, Na_3PS_4 and its derivatives offer promising ionic conductivities [2]. Na_3PS_4 and Na_3PSe_4 both crystallize in a tetragonal phase (*P-421c*) at low temperature and transform to a cubic phase (*I*-43*m)* around 530K and 270K, respectively[3-6], which exhibits high ionic conductivity of order mS/cm [3,5]. We have

performed the quasielastic (QENS) and inelastic neutron scattering (INS) measurements to probe the Na diffusion dynamics and the potential role of phonons in facilitating the fast diffusion process. The QENS and INS measurements were performed using the BASIS and ARCS spectrometers at the Spallation Neutron Source. Our neutron scattering measurements, complemented with our ab-initio molecular dynamics (AIMD) simulations and anharmonic first-principles phonon simulations, enable us to determine the jump like diffusion mechanism of Na. We identify strongly anharmonic low-energy phonon modes involving PX_4 units, which couple to Na diffusion. The QENS measurements and AIMD simulations show that Na ions hop between octahedral sites (6b Wycoff site), with jump length and residence time d_{jump}~3.5 Å and t_{res}~500 ps. Large diffusion coefficients are estimated using a Chudley Elliot jump diffusion model and are attributed to a soft lattice, and PX4 liberational modes, in particular in Na_3PSe_4. The simulations also reveal strongly correlated motions of Na ions along 1D chains in both compounds. Our combined experiments and simulations also enable us to quantify the importance of ionic correlations and coherent scattering effects in QENS analysis.

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PB.01.18

Probing Intraparticle and Interparticle Magnetic Structures in Chemically Homogeneous Manganese Ferrite Nanoparticle Assemblies

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Magnetic nanoparticles are central to many important biomedical and sensor applications, but it is challenging to identify the governing intraparticle and interparticle interactions that influence their behavior. In recent work, we have shown that dense core-shell $Fe_3O_4/Mn_xFe_{3-x}O_4$ ($x \sim 1$) nanoparticle assemblies can display not only an interesting canted spin structure within a particle but one which is correlated from nanoparticle to nanoparticle [1,2]. The extended structures are explained via a simple model considering structural stacking faults in the nanoparticle packing and the resulting influence on interparticle dipolar interactions. However, the complex chemical structure of these particles makes it difficult to distinguish the explicit role of other underlying terms like exchange and Dzyaloshinskii-Moriya interactions; it is also unclear how critical the core-shell morphology is to the observed spin correlations. Here, we discuss our recent preliminary results studying dense ordered assemblies of 7.6 nm diameter chemically homogeneous $MnFe_2O_4$ nanoparticles, where special care has been taken with the precursor materials in a standard preparation method [3] to assure chemical uniformity throughout the particles. The particle assemblies have been investigated using polarization-analyzed small angle neutron scattering (PASANS) methods to allow for clean separation of magnetic vs. structural features. The experiments were performed at the newly developed 45 m very small angle neutron scattering (vSANS) instrument at the NIST Center for Neutron Research which allows for a wide Q range (~0.005 to 0.15 $Å^{-1}$) to be measured simultaneously, greatly improving data-taking efficiency. Full four cross-section polarization data were collected on the particle assemblies for a range of temperatures (10-410 K) and magnetic fields (0 to 1.4 T). While the magnetic behavior in remanence mostly follows a single particle form factor, the scattering deviates and grows maximally at intermediate temperatures (~50-100 K). In addition, the variation of the angular dependence of the spin-flip scattering differs from that expected for isotropic spin canting, indicating a rich magnetic morphology with field and temperature. These results highlight the ability of PASANS to extract important magnetic features in nanoscale systems.

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PB.01.19

High Temperature Non-Harmonic Phonons of Chromium from Inelastic Neutron Scattering and *Ab Initio* Calculations

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In this study, we measured phonon densities of states (DOS) of bcc chromium from 6-1493 K using ARCS,

a high flux direct geometry neutron spectrometer, and compared them to *ab-initio* density functional theory (DFT) calculations within both a quasi-harmonic approximation and a temperature-dependent effective potential (TDEP) framework. The observed energies of the transverse mode over this temperature range exhibit an abnormal softening of approximately 12%. The quasi-harmonic approximation, where phonon spectra are assumed to be solely volume dependent, is unable to capture this shift. Nonmagnetic TDEP calculations, which include both volume and explicit temperature effects on phonon energies, reflect this softening. Using the connection between vibrational densities of states and high temperature thermodynamics, we compute thermal expansion, entropy, and heat capacity at high temperature. Our computational results contrast with a recent study which proposed that strong magnetic coupling in Cr is responsible for the observed high temperature calorimetric data rather than pure anharmonicities [4]. When comparing the entropy calculated from the measured phonon DOS to the calorimetric entropy of Cr, we found excellent agreement at temperatures below 600 K. At higher temperatures, however, there seems to be an additional contribution to the calorimetric entropy. A similar discrepancy was noted in a previous computational study [4]. We help assess this disagreement using the above phonon-phonon interactions (TDEP) and also consider the contribution of electron-phonon interactions to the thermodynamics of Cr.

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PB.01.20
Polarized Neutron Scattering of $FeTe_{1-x}Se_x$ - Magnetism and Electronic Coherence
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Local inhomogeneity has a great impact on the electronic band structure and magnetic properties of correlated quantum materials. We apply polarized neutron spectroscopy, together with spatially-resolved chemical and electrical analysis, to a topological superconductor candidate, $FeTe_{1-x}Se_x$. The detailed physical and chemical information points to an underlying connection among magnetism, electronic coherence, and superconductivity. Work at Brookhaven is supported by the Office of Basic Energy Sciences, Materials Sciences and Engineering Division, U.S. Department of Energy (DOE) under Contract No. DE-SC0012704.

PB.01.21
Neutron Diffraction Investigation on Y-Type Hexaferrites
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The discovery of magnetoelectric (ME) effects caused by a cycloidal spin order has initiated intense research on the new class of ME materials [1]. Among them, one interesting class of materials is the Y-type hexaferrite (A2Me2Fe12O22: Me=transition metal)[2]. These materials are being extensively investigated because they exhibit spin-driven ferroelectricity associated with non-collinear magnetic structures in the relatively low magnetic field and high-temperature region [3,4]. The Y-type hexaferrite BaSrCo2Fe11AlO22 was recently reported to exhibit spin-driven ferroelectricity and electric-field induced magnetization switching at room temperature [5]. The ME properties of Y-type hexaferrite are dominated mainly by the so-called FE3 phase via the spin-driven electric polarization. At the same time the electric-field-active magnetic excitations, which is referred to as electromagnon have been observed in this Y-type hexaferrite[6], similar to the electromagnon in another Y-type hexaferrite Ba2Mg2Fe12O22 [7,8,9]. In this presentation we report on the recent neutron diffraction investigation on (Ba2-ySry)Co2Fe12-x AlxO22 , x=0.9 with different Sr-doping of y=0.8,1.0 and 1.2. Combined with magnetization and electric polarization measurements, the H-T magnetic phase diagrams are revealed. The stability of the multiferroic FE3 phase is greatly improved in the Sr-rich compound. While the FE3 phase in the Ba-rich compound (y=0.8) is fragile against the removal of the magnetic field at room temperature, it is robust in the Sr-rich compound (y=1.2), even against zero-field cooling [10].

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PB.01.22

Magnetic Properties of the Doped Mott Insulator $YTiO_3$

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The transition metal oxides $RTiO_3$, where R is a trivalent rare-earth ion, are typical Mott-Hubbard insulators, with the Ti ion in the $3d^1$ configuration. The observed $GdFeO_3$ -type tilt distortion of the TiO_3 octahedra controls the electron transfer between the Ti 3d and O 2p orbitals, and hence constitutes a bandwidth-control mechanism. The end members $YTiO_3$ and $LaTiO_3$ of this series exhibit large and small distortions, respectively, with Ti-O-Ti bond angles of 140 and 156 degrees. Consequently, the physical properties across the $RTiO_3$ series exhibit significant variation dependent on the rare-earth ion, as $YTiO_3$ is a ferromagnetic (FM), whereas LaTiO3 is an ntiferromagnetic (AFM). In both cases, hole doping induces a metallic state; the insulator-metal transition (IMT) in $Y_{1-x}Ca_xTiO_3$ and $La_{1-x}Sr_xTiO_3$ occurs at significantly different concentrations of x=0.37 and y=0.05, respectively [1]. The robust insulating state of $YTiO_3$ makes the system particularly interesting, notwithstanding various other peculiarities, as it has been argued that orbital order is responsible for the ferromagnetic ground state. Here we report elastic and inelastic neutron scattering results for $Y_{1-x}La_xTiO_3$ and hole-doped $Y_{1-x}Ca_xTiO_3$, with focus on the spin-wave spectrum and magnetic order parameter. The results help to elucidate the respective evolution from FM to AFM insulator and FM insulator to paramagnetic metal. The work at the University of Minnesota was funded by the Department of Energy through the University of Minnesota Center for Quantum Materials, under Grant No. DE-SC-0016371.

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PB.01.23

High Pressure Neutron Scattering Studies of the Plaquette State of the Shastry-Sutherland Compound $SrCu_2(BO_3)_2$

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The Shastry-Sutherland compound $SrCu_2(BO_3)_2$ features 2D layers of Cu^{2+} S=1/2 spin dimers which are orthogonal to each other. The ground state of the system is determined by the relative strength of the nearest neighbor and next-nearest neighbor interactions, J and J' respectively. The ratio of J/J' can be tuned continuously by application of hydrostatic pressure. The ground state changes from a spin dimer singlet state at ambient pressure to an antiferromagnet state at high pressure. At intermediate pressure a novel 4-spin plaquette singlet state has recently been reported. However, the nature of this plaquette state and how it evolves into other phases remains unclear. Here, we report a comprehensive study of the quantum phase diagram of the plaquette state by tuning temperature, pressure, magnetic field, and chemical doping. We mapped out the evolution of the ground states using complementary techniques such as magnetization measurements and neutron scattering. The results provide insights into the nature of the plaquette state, and also has implications in areas such as studies of deconfined quantum criticality.

PB.01.24
Neutron Scattering Studies of Tm-Based Breathing Pyrochlore System
Lalit Yadav[1], Rabindranath Bag[1], Sachith Dissanayake[1], Zhenzhong Shi[1], Guangyong Xu[2], Hui Wu[2], Craig M. Brown[2], Nicholas Butch[2], Franz Lang[3], Stephen blundell[3] and Sara Haravifard[1,1]; [1]Duke University, United States; [2]Center of Neutron Research, National Institute of Standards and Technology, United States; [3]University of Oxford, United Kingdom

Breathing Pyrochlore materials have emerged as a promising candidate to study frustrated magnetism and topological magnons. We have initiated the design and synthesis of rare-earth based Breathing Pyrochlore compounds. Further, we have been using neutron diffraction and inelastic neutron scattering techniques to probe the static and dynamic properties of these compounds. In this talk, we are going to present our latest experimental results for the Tm-based breathing pyrochlore compound Ba3Tm2Zn5O11.

PB.01.25
Field Dependent Neutron Scattering Studies of Breathing Pyrochlore $Ba_3Yb_2Zn_5O_{11}$
Sachith Dissanayake[1], William M. Steinhardt[1], Zhenzhong Shi[1], Stephen Kuhn[1], Jeff Rau[2], Nicholas Butch[3], Matthias D. Frontzek[4], Andrey Podlesnyak[4], Yiming Qiu[3], Wangchun Chen[3], David Graf[5], Tao Hong[4], Casey Marjerrison[1], Michel Gingras[6] and Sara Haravifard[1,1]; [1]Duke University, United States; [2]University of Windsor, Canada; [3]National Institute of Standards and Technology, United States; [4]Oak Ridge National Laboratory, United States; [5]National High Magnetic Field Laboratory and Department of Physics, Florida State University, United States; [6]University of Waterloo, Canada

Breathing pyrochlore systems are composed of corner-sharing tetrahedra of different sizes pointing in opposing directions, leading to different intra- and inter-tetrahedra exchange interactions and the emergence of the Dzyaloshinskii-Moriya interaction due to loss of inversion symmetry. They are predicted to host exotic physics including quantum spin ice, quantum spin liquid, and field-tunable topological magnons. Here we will present single-crystal field-dependent unpolarized and polarized inelastic neutron scattering measurements on Yb-based breathing pyrochlore system, as well as a theoretical model that can effectively describe some of our experimental findings.

PB.01.26
Synthesis and Characterization of a Rare-Earth Based Triangular Borate Family
Rabindranath Bag[1], Matthew Ennis[1], Sachith Dissanayake[1], Zhenzhong Shi[1], Alexander I. Kolesnikov[2], Hui Wu[3], Craig M. Brown[3], David Graf[4] and Sara Haravifard[1,1]; [1]Duke University, United States; [2]Oak Ridge National Laboratory, United States; [3]National Institute of Standards and Technology, United States; [4]National High Magnetic Field Laboratory, United States

Geometrically frustrated magnets are considered one of the most interesting topics in condensed matter physics due to a variety of exciting physics such as quantum spin liquid, spin glass and spin ordered state. Rare-earth based borate family having two dimensional (2D) triangular lattice structure is a good candidate to host many exotic ground states. We have successfully synthesized and grown the centimetric size single crystals of a series of borate compounds with different rare earth elements. Low temperature static properties of rare-earth based borates are performed using neutron diffraction while crystalline electric field levels are identified using inelastic neutron scattering technique. In this talk, I will present our latest results achieved from the synthesis and advanced characterization experiments.

PB.01.27
Anharmonic Effects on Phonon Eigenvectors and *S(Q,E)* in Quantum Paraelectric $SrTiO_3$
Xing He[1], Dipanshu Bansal[2], Barry Winn[3], Songxue Chi[3], Lynn Boatner[3] and Olivier Delaire[1]; [1]Duke University, United States; [2]Indian Institute of Technology Bombay, India; [3]Oak Ridge National Laboratory, United States

The quantum paraelectric behavior and strongly anharmonic lattice dynamics of $SrTiO_3$ have attracted interest for decades. Reflecting the incipient ferroelectric instability near the quantum critical point and anharmonic couplings between acoustic and optic phonons, anomalous temperature-dependent phonon intensities were observed in multiple Brillouin zones (BZs) from inelastic neutron scattering (INS) experiments on $SrTiO_3$. The Hybrid Spectrometer (HYSPEC) and HB3 triple-axis spectrometer at Oak Ridge National Laboratory (ORNL) were used to track phonon intensities over a wide temperature range and for a large volume in reciprocal space. The *S(**Q**,E)* data reveal a strong softening of the zone-center transverse optic (TO) mode, congruent with incipient ferroelectricity (FE), and simultaneously a strongly anomalous evolution of the intensity of transverse acoustic (TA) modes, which decreases dramatically on cooling. The experimentally observed trends are confirmed and rationalized using ab initio molecular dynamics

(AIMD) and anharmonically renormalized phonon methods, which achieve quantitative agreement with the INS experiments. By analyzing the simulated temperature-dependent force-constants (FC) and eigenvectors, it is found that the structure factors $|F|^2$ of TA and TO modes change dramatically with temperature, as a direct consequence of the strong anharmonicity in this system. Moreover, we identify that the changes of Ti and O eigenvectors are responsible for these striking observations, which originates from Ti-O inter-atomic FC changing with temperature. These results establish how temperature-dependencies of phonon intensities beyond the harmonic picture can be quantitatively measured through INS mapping of $S(\boldsymbol{Q}, E)$ volumes, providing direct insights into the behavior of phonon eigenvectors in real space, and also show how first-principles simulations including anharmonic effects can reproduce and rationalize such anharmonic effects [1]. This work was supported by the U.S. DOE.

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PB.01.28

Neutron Scattering Studies of Triangular Antiferromagnet YbZnGaO4

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In the last few years YbMgGaO4 and related triangular antiferromagnets emerged as promising quantum spin liquid candidates, and subsequently their ground states have been the subject of ardent debates. Though many experimental and theoretical studies have been devoted to investigating the magnetic properties of these systems at very low temperatures, and exploring a range of possible explanations for the observed spin liquid-like phenomena, a definitive description remains elusive mainly due to chemical disorder. In this presentation we discuss neutron scattering experiments in applied magnetic fields to probe static and dynamic properties of YbZnGaO4.

PB.01.29

Neutron Scattering Studies of Yb-Based Triangular Borate

Matthew Ennis[1], Sachith Dissanayake[1], Rabindranath Bag[1], Zhenzhong Shi[1], Alexander I. Kolesnikov[2], Jose A. Rodriguez-Rivera[3], Nicholas Butch[3], Hui Wu[3], Craig M. Brown[3] and Sara Haravifard[1,1]; [1]Duke University, United States; [2]Oak Ridge National Laboratory, United States; [3]National Institute of Standards and Technology, United States

Recently, triangular antiferromagnetic materials have attracted attention because competing interactions on the lattice can give rise to exotic phenomena, such as quantum spin liquids. We have initiated systematic efforts to synthesize single crystal samples of a family of rare-earth based triangular antiferromagnet double borates. In particular, focus has been given to one member of this family, Ba3Yb(BO3)3 (BYBO), which features spin-½ ytterbium ions on a triangular lattice. We have conducted neutron scattering studies on both powder and single crystal samples of BYBO to probe the static and dynamic properties of this system. In this talk, we will present the results of our experimental efforts.