MA 19: Magnetic Materials III

Time: Tuesday 11:30–13:15 Location: H31

MA 19.1 Tue 11:30 H31

Exchange interactions and Curie temperatures in tetrametal nitrides Cr4N, Mn4N, Fe4N, Co4N, and Ni4N — •Markus Meinert — Center for Spinelectronic Materials and Devices, Bielefeld University, Germany

The tetrametal nitrides exhibit a surprising relation between total magnetic moments, site-resolved magnetic moments and Curie temperatures. In Mn_4N, the Curie temperature is rather high, whereas the Curie temperatures of Fe_4N and Ni_4N are comparatively low.

Ab-initio calculations of the exchange interactions and classical Monte Carlo simulations of the temperature dependent magnetizations were performed to understand the observed relations. It turns out that the calculations reproduce the observed magnetic moments and Curie temperatures very well. The fact that the Curie temperature of Fe_4N is not higher than 760K in spite of the high magnetic moment (2.4 μ_B per Fe atom) can be traced back to an antiferromagnetic intrasublattice interaction between Fe atoms on the unit cell faces, which destabilizes the ferromagnetic order.

MA 19.2 Tue 11:45 H31

First-principles investigation of the magnetic properties of $Fe_{1/4}NbSe_2$ — •H. Kouarta[1,2], J. Ibanez-Azpiroz[1], M. dos Santos Dias[1], S. Lounis[1], and H. Belkhir[2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany — [2]Laboratoire d'Etudes des Surfaces et Interfaces du solide, Département de Physique, Faculté des Sciences, Université Badji Mokhtar, BP 12, 23000, Annaba, Algeria

We investigated from first-principles the intercalated transition metal dichalcogenide $Fe_{1/4}NbSe_2$ using the full-potential augmented plane waves and the Korringa-Kohn-Rostoker Green function methods. We explored the different possible magnetic states with a focus on the possibility to find Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions since the latter were proposed to occur in a similar material: $Fe_{1/4}TaS_2$[1]. The ground state is of antiferromagnetic nature, where the Fe spin magnetic moments were found to be smaller ($2.82\mu_B$) than the measured values ($4.9\mu_B$)[2]. Our analysis highlights the strong/weak hybridization between Fe 3d and Se 4p/Nb 4d states. Correlation effects in terms of an on-site Coulomb interaction U increased the moment by ~ 0.5 μ_B. With the spin-orbit interaction considered, an orbital moment of 0.6 μ_B was computed bringing the total Fe magnetic moment to 4 μ_B in a closer agreement with the experiment.

[1]K.-T.Ko et al., Phys. Rev. Lett, 107,247201 (2011); [2]S. S. P. Parkin and R. H. Friend, Philos. Mag. B 41, 65 (1980).

MA 19.3 Tue 12:00 H31

Magnetic anisotropy in MAX Phases — •Ruslan Salikhov[1], Ulf Wiedwald[1], Arni S. Ingason[2], Johanna Rosen[2], and Michael Farle[1] — [1]University Duisburg-Essen, Duisburg, Germany — [2]Linköping University, Linköping, Sweden

MAX phases (Mn+1AXn, where n = 1, 2, or 3) are ternary compounds consisting of an early transition metal M (including Mn), an A-group element A, and either C or N, denoted X. MAX phases have attracted considerable interest due to unique material properties combining properties usually associated with metals (electrically and thermally conductive) and ceramics (lightweight, stiff and resistive against oxidation) [1]. The crystal structure of MAX phases is hexagonal with repeated M-X-M (quasi 2D) atomic layers stacking in the c-direction with the A-element as a spacer. The recently discovered magnetic MAX phases (Cr0.5Mn0.5)2GaC and (Cr0.6Mn0.4)2GeC [2, 3] were prepared as epitaxial films and studied by ferromagnetic resonance (FMR) and SQUID magnetometry. We find that the (Cr0.5Mn0.5)2GaC film has a negligibly small magnetocrystalline anisotropy energy density (MAE) and the spectroscopic splitting factor is 2.00 +- 0.02 [4]. The (Cr0.6Mn0.4)2GeC film, however, shows a high MAE of 0.1 MJ/m3 at T = 100 K with the easy axis parallel to the c axis (perpendicular to the film plane).

[1] M. W. Barsoum, Prog. Solid State Chem. 28, 201, (2000).
[2] A. Petruhins et al., Journal of Materials Science 50, 4495 (2015).
[3] A. S. Ingason et al., Phys Rev Lett. 110, 195502 (2013).
[4] R. Salikhov et al., Mater. Res. Lett. 3, 156 (2015).

MA 19.4 Tue 12:15 H31

Resonant inelastic x-ray scattering of magnetic excitations in the novel 5d^4 iridate Ba_2YIrO_6 — •Maximilian Kusch[1], Tusharkanti Dey[1], Andrey Malyuk[1], Sabine Wurmehl[1], Bernd Büchner[1,2], Vamshi Katukuri[3], Beom Hyun Kim[5], Dmitry Efremov[3], Jeroen van den Brink[3], Marco Moretti[4], Michael Krisch[4], and Jochen Geck[1] — [1]Institute for Solid State and Materials Research, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Institut für Festkörperphysik, Technische Universität Dresden D-01062 Dresden, Germany — [3]Institute for Theoretical Solid State State Physics, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [4]European Synchrotron Radiation Facility, B.P.220, 38043 Grenoble, France — [5]Pohang university of science and technology

Ba_2YIrO_6 is a realization of a Ir-5d^4 electronic configuration forming a $J = 0$ ground state. Recently they gained particular interest since theoretical studies proposed, that a new type of van-Vleck like paramagnetism including excitation of non-zero J (J = 1, 2) might play an important role [khaliullin2013]. Our theoretical model calculations of the momentum dependence of these excitations predict a considerable dispersion of the J=1 and J=2 excitations and, in dependence on model parameters, a dramatic softening of excitations is observed. We performed high-resolution resonant inelastic x-ray scattering (RIXS) studies on Ba_2YIrO_6 to determine these dispersions experimentally. The results of these measurements are presented and discussed in comparison to the model calculations.

MA 19.5 Tue 12:30 H31

Interplay of structure and magnetism in frustrated intermetallic AFe_4X_2 systems — •Inga Kraft[1,2], Katharina Weber[1,2], Christoph Bergmann[1], Nandang Mufti[1], Til Goltz[2], Hans-Henning Klauss[2], Christoph Geibel[1], and Helge Rosner[1] — [1]Max Planck Intitute for Chemical Physics of Solids, Dresden — [2]Technical University of Dresden

Due to their complex and versatile behavior frustrated systems present a great experimental and theoretical challenges. Even slight perturbations induce instabilities in such systems and prompt the emergence of unusual phenomena. The intermetallic AFe_4X_2 compounds (A=Sc,Y,Lu,Zr; X=Si,Ge) are suggested to cover the whole regime from frustrated AFM order up to an AFM quantum critical point. Our DFT calculations exhibit a strong interplay of structure and magnetism. We discuss the influence of the A and X site atoms on the strength of magnetic interactions and the size of structural distortion.

MA 19.6 Tue 12:45 H31

Study of the magnetic excitation spectrum of the helimagnetic spinel compound $ZnCr_2Se_4$ — •Alistair Cameron[1], Yullia Tymoshenko[1], Yevhen Onykiienko[1], Pavlo Portnichenko[1], Helen Walker[2], Douglas Abernathy[3], and Dmytro Inosov[1] — [1]Institut für Festkörperphysik, TU Dresden, Germany — [2]ISIS Neutron Source, Rutherford Appleton Laboratory, United Kingdom — [3]SNS, Oak Ridge National Laboratory, United States

$ZnCr_2Se_4$ is a magnetoelectric compound with a cubic spinel ($Fd\bar{3}m$) structure. In zero applied field, the Cr^{3+} S=3/2 moments form an incommensurate magnetic ground state with a screw structure along the [100] direction and a T_N of 20 K, which transforms into a spin-spiral state in an applied magnetic field. Above the critical field H_{C2} this material exhibits a proposed spin-nematic state, before becoming fully ferromagnetic at H_{C3}. Previously, we studied this material with neutron diffraction, and found a temperature- and field-dependent magnetic structure in the spin-spiral phase with no long-range order in the proposed spin-nematic state. Here, we probe the spin-excitation spectrum of $ZnCr_2Se_4$ using time-of-flight neutron scattering, which allows us to investigate a large area of momentum space. The relatively short spin-spiral in $ZnCr_2Se_4$ leads to a large separation of the nuclear and magnetic Brag peaks in momentum space, making it possible to resolve excitations originating from a single magnetic Bragg peak. We observe two clear branches emanating from the magnetic satellites, an intense low energy mode alongside a steeper, less intense branch at higher energies.

MA 19.7 Tue 13:00 H31

Study of the geometrically frustrated compound $Nd_2Sn_2O_7$
— •Bertin A.[1], Dalmas de Réotier P.[2,3], Fåk B.[4], Marin C.[2,3], Yaouanc A.[2,3], Forget A.[5], Sheptyakov D.[6], Frick B.[4], Ritter C.[4], Amato A.[7], Baines C.[7], and King P.J.C.[8] — [1]TU Dresden — [2]Univ. Grenoble Alpes — [3]CEA-Grenoble, INAC-SPSMS — [4]Institut Laue-Langevin — [5]CEA-Saclay, Iramis, SPEC — [6]Paul Scherrer Institute, SINQ — [7]Paul Scherrer Institute, SμS — [8]ISIS Facility, Rutherford Appleton Laboratory

We have undertaken the study of the antiferromagnet pyrochlore compound $Nd_2Sn_2O_7$ where frustration lattice consists of magnetic ions sitting on a corner-shared tetrahedra network. This compound undergoes a second-order phase transition at $T_c = 0.91$ K into a non collinear "all-in-all-out" magnetic structure, confirmed by the presence of spontaneous oscillations resolved with zero-field μSR measurements. Persistent spin dynamics has been revealed through the temperature independent behaviour of the spin-lattice relaxation rate at low temperatures, and ascribed to 1-dimensional spin-loop excitations. This feature, together with the spin-wave-like excitations seen by specific heat measurements at low temperatures, are barely compatible with a purely Ising spin system and point to the existence of transverse exchange terms. Hence, the anisotropic Hamiltonian for dipolar-octupolar doublet will be discussed. Anomalously long paramagnetic fluctuations have also been revealed by μSR and neutron backscattering experiments up to $\approx 30\ T_c$. The funding of the current position of the presenting author by BMBF project 05K13ODA is acknowledged.