MA 24: Molecular Magnetism II

Time: Wednesday 9:30–11:00 Location: HSZ 02

MA 24.1 Wed 9:30 HSZ 02

Studies of decoherence in strongly anisotropic spin triangles with toroidal or general non-collinear easy axes — Kilian Irländer and •Jürgen Schnack — Universität Bielefeld, Bielefeld, Deutschand

Magnetic molecules are investigated with respect to their usability as units in future quantum devices. In view of quantum computing, a necessary prerequisite is a long coherence time of superpositions of low-lying levels. In this article, we investigate by means of numerical simulations whether a toroidal structure of single-ion easy anisotropy axes is advantageous as often conjectured. Our results demonstrate that there is no general advantage of toroidal magnetic molecules, but that arrangements of tilted anisotropy axes perform best in many cases.

MA 24.2 Wed 9:45 HSZ 02

Electrically driven singlet-triplet transition in triangulene spin-1 chains — Gabriel Martínez-Carracedo[1,2], •László Oroszlany[3,4], Amador García-Fuente[1,2], László Szunyogh[5,6], and Jaime Ferrer[1,2] — [1]Universidad de Oviedo, Oviedo, Spain — [2]CINN, Universidad de Oviedo-CSIC, El Entrego, Spain — [3]Eotvos Lorand University, Budapest, Hungary — [4]MTA-BME Lendulet Topology and Correlation Research Group, Budapest University of Technology and Economics, Budapest, Hungary — [5]Budapest University of Technology and Economics, Budapest, Hungary — [6]ELKH-BME Condensed Matter Research Group, Budapest University of Technology and Economics, Budapest, Hungary

Recently, graphene triangulene chains have been synthesized and their magnetic response has been analyzed by STM methods by Mishra and coworkers (Nature 598, 287 (2021)). Motivated by this study, we determine the exchange bilinear and biquadratic constants of the triangulene chains by calculating two-spin rotations in the spirit of the magnetic force theorem. We then analyze open-ended, odd-numbered chains, whose edge states pair up forming a triplet ground state. We propose three experimental approaches that enable us to trigger and control a singlet-triplet spin transition. Two of these methods are based on applying a mechanical distortion to the chain. We finally show that the transition can be controlled efficiently by the application of an electric field.

MA 24.3 Wed 10:00 HSZ 02

Linear magnets: a structure-property-relation for finding unquenched orbital moments — •Anton Jesche — EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86135 Augsburg, Germany

The presence of orbital magnetic moments in rare-earth-elements is one of the major differences to transition metal compounds and is at the heart of magnetic anisotropy, stability, and functionality. A large crystal electric field effect acting on an unquenched orbital moment can lead to extremely large anisotropy and coercivity as experimentally verified for iron-doped lithium nitride [1]. In the dilute limit, those iron atoms can be considered as single-atom magnets and are ideal candidates to study the quantum dynamics of anisotropic spins [2,3]. This, together with the strong field dependence of the spin reversal, allows the creation of stable but switchable states that could act as a 'quantum bit' at elevated temperatures of 10 K. A recent Mössbauer study revealed dominant magnetic quantum tunneling at even higher temperatures [4]. The presence of orbital moments in iron-doped lithium nitride is not a coincidence and not a solitary case: based on the proposed structural motif of the 'linear chain', we have identified several other 'linear magnets' with similar physical properties: iron-doped Li4SrN2, LiSr2(CoN2), and (Sr6N)[FeN2][CN2]2. Implications and limitations of linear coordination are discussed in relation to the electronic structure. [1] M. Fix et al. PRB 97, 064419 (2018) [2] M. Fix et al. PRL 120, 147202 (2018) [3] M. Huzan et al. Chem. Sci. 11, 11801 (2020) [4] S. A. Bräuninger et al. PRB 102, 054426 (2020)

MA 24.4 Wed 10:15 HSZ 02

Modelling of saw-tooth chain molecules composed of 3d and 4f ions — •Dennis Westerbeck and Jürgen Schnack — Universität Bielefeld, D-33501 Bielefeld, Deutschland

Metal- and lanthanide-ion containing systems are of great interest for the investigation of the magnetic properties of molecular systems. Especially the gadolinium containing systems are promising in view of magnetocaloric applications. In addition, saw-tooth like systems are considered as favorable for low-temperature cooling due to their massively degenerate ground-state. Although Fe^{III} and Gd^{III} are mostly considered as isotropic in multi-ion systems, we show that zero-field splittings are inevitable for the proper description of some of these molecules. Furthermore, these anisotropic saw-tooth systems show a significant isothermal entropy change, which is surprisingly well described by our simulations.

MA 24.5 Wed 10:30 HSZ 02

High-field/high-frequency EPR studies on heterometallic 3*d*-4*f*-complexes — •Jan Arneth[1], Changyun Koo[1], Xiangfeng Li[2], Annie K. Powell[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Institute of Inorganic Chemistry, Karlsruhe Institute of Technology, Germany

On the road to the construction of novel efficient single molecular magnets and molecular magnetic refrigerants experimental investigation of the exchange coupling mechanism between $4f$ and $3d$ moments is an important, yet still challenging, task. The difficulty in understanding the rich physics underlying this coupling arises from the strong participation of orbital angular momentum leading to large anisotropy and a complex energy spectrum in $4f$ metal compounds. Here, we present high-field/high-frequency electron paramagnetic resonance (HF-EPR) studies on heterometallic $3d$-$4f$ complexes with so-called butterfly motif Fe_2Ln_2 (Ln = Y, Gd, Dy), V_2Ln_2 (Ln = Er, Ho) and in the saw-tooth coordination V_4Ln_4 (Ln = La, Gd), which allow us to directly determine not only the exchange coupling constants but also other spin-hamiltonian parameters, such as g-values and anisotropy. Our spectroscopic measurements are further complemented by high-field magnetisation studies.

MA 24.6 Wed 10:45 HSZ 02

AOM-guided Linked Fits for Analysing Inelastic Neutron Scattering and Magnetic Data of 3*d*-4*f* Heterometallic M_2Ln_2 Single-Molecule Magnets — •Julius Mutschler[1], Thomas Ruppert[2], Yan Peng[2], Jacques Ollivier[3], Quentin Berrod[3], Jean-Marc Zanotti[3], Christopher E. Anson[2], Annie K. Powell[2], and Oliver Waldmann[1] — [1]Physikalisches Institut, Universität Freiburg, D-79104 Freiburg, Germany — [2]Institut of Inorganic Chemistry, Karlsruhe Institute of Technology (KIT), D-76131 Karlsruhe, Germany — [3]Institut Laue-Langevin, F-38042 Grenoble Cedex 9, France

The discovery two decades ago of slow relaxation and quantum tunnelling of the magnetization in the single molecule magnets (SMMs) has inspired a flurry of research into their magnetic properties. This class of molecules has been extended to heterometallic clusters containing ions of transition metals and rare earths. The $4f$ ions are of interest because of their large angular momentum and magnetic anisotropies, but also present challenges in the analysis of inelastic neutron scattering (INS) and magnetic data. As presented in the previous meeting, excellent INS data were recorded on the time-of-flight disk-chopper spectrometers IN5 and IN6 at ILL on the Mn_2Ln_2-squares with Ln = Y, Tb, Ho, Dy, and the M_2Ln_2-butterflies with M = Fe, Al and Ln = Dy, Er. In this talk, the analysis of the complete set of magnetic data using an AOM-guided linked fit is presented. The resulting ligand field and coupling parameters give crucial hints for the analysis of the rich INS spectra.