MA 28: Bio- and molecular magnetism including biomedical applications

Time: Wednesday 9:30–11:30 Location: H52

MA 28.1 Wed 9:30 H52

Magnetite-gold nanoparticles: from physics to theranostics — •Maria V. Efremova[1,2], Yulia A. Nalench[2], Eirini Myrovali[3], Anastasiia S. Garanina[1,2], Victor A. Naumenko[2], Maxim A. Abakumov[2,4], Marina Spasova[5], Michael Farle[5], Alexander G. Majouga[1,2,6], Natalia L. Klyachko[1,2], and Ulf Wiedwald[2,5] — [1]MSU, Moscow, Russia — [2]NUST MISIS, Moscow, Russia — [3]AUTH, Thessaloniki, Greece — [4]RNRMU, Moscow, Russia — [5]UDE, Duisburg, Germany — [6]MUCTR, Moscow, Russia

In this work, we prepare pairwise connected $Fe_3O_4 - Au$ hybrid nanoparticles (NPs) with diameters of 6-44 nm Fe_3O_4 and 3-11 nm Au aiming for optimized theranostics response in magnetic particle hyperthermia (MPH) and magnetic resonance imaging (MRI).

With increasing NPs diameter from 6 to 25 nm in agarose mimicking tissues, the MPH reveal that the specific loss power increases from 12 to 327 W^*gFe^{-1}, while for the MRI, we observe the growth of the r_2-relaxivity from 118 to 612 $mM^{-1}s^{-1}$. The 25 nm and 44 nm diameter NPs show the similar theranostic performance. These values are significantly enhanced in comparison to other $Fe_3O_4 - Au$ hybrids due to their octahedral shape and large M_s. As a practical application, MRI-controlled drug delivery and dual-mode MRI/fluorescent imaging are presented for the optimized NPs size of 25 nm.

The reported study was funded by the Russian Foundation for Basic Research 18-33-01232 (fluorescent labeling of NPs) and Increase Competitiveness Program of NUST MISIS K3-2017-022 (magnetic measurements).

MA 28.2 Wed 9:45 H52

Superparamagnetic Magnetic Nanoparticle Detection for Early Diagnosis of Neurodegenerative Diseases — •Luca Marnitz, Anastasiia Moskaltsova, Jan Schmalhorst, and Günter Reiss — Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld

This talk will introduce a new technique for the early detection of neurodegenerative diseases developed within the H2020 project MADIA [1]. It will focus on the development and integration of magnetoresistive sensors which are able to detect small amounts of superparamagnetic magnetic nanoparticles (SMNPs) with diameters of about 50nm inside a microfluidic channel. For this purpose, sensors based on the Giant Magnetoresistance (GMR), Tunneling Magnetoresistance (TMR) and Planar Hall Effect (PHE) were evaluated regarding their suitability for this purpose. The specific challenges of integrating the sensors in microfluidic lab-on-chip systems will be discussed and the realized solutions will be presented. [1]http://www.madia-project.eu/

MA 28.3 Wed 10:00 H52

Time-dependence of fundamental thermodynamic processes investigated in anisotropic magnetic molecules — •Christian Beckmann and Jürgen Schnack — Bielefeld University, Universitätsstr. 25, 33615 Bielefeld

The theoretical understanding of time-dependence in magnetic quantum systems is of great importance in particular for cases where a unitary time evolution is accompanied by relaxation processes. This is of special interest for the realization of fundamental thermodynamic processes.

In this contribution we investigate how a fundamental thermodynamic process, such as the Carnot process, can be performed with finite velocity on an anisotropic magnetic molecule by rotation of the applied magnetic field.

MA 28.4 Wed 10:15 H52

Magnetism of highly-ordered Fe_4 single molecule magnets on a superconductor — •Fabian Paschke[1], Vivien Enenkel[1], Michal Studniarek[2], Jan Dreiser[2], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universitaet Konstanz, 78457 Konstanz, Germany — [2]Swiss Light Source, Paul Scherrer Institute, 5232 Villigen, Switzerland

The controlled deposition, characterization and manipulation of single molecule magnets (SMMs) on surfaces is one of the crucial investigation topics with regard to their possible implementation as units in future electronic and spintronic devices. Fe_4 derivatives are among the most investigated SMMs showing a giant spin and a variety of quantum mechanical phenomena [1]. We recently employed inelastic electron tunneling spectroscopy (IETS) on single molecules to confirm the retained molecular magnetism upon deposition on the isolating graphene surface [2,3].

Here we present the successful deposition and investigation of Fe_4H SMMs on superconducting Pb(111). Using scanning tunneling microscopy (STM) and spectroscopy (STS) we reveal a highly-ordered self assembly of intact Fe_4H molecules and deduce the electronic molecule-substrate interaction by measuring HOMO and LUMO resonances. Magnetic exchange interaction and anisotropy are accessed by IETS and XMCD measurements, revealing the influence of the superconducting Pb surface on the molecular magnetism.

[1] C. Cervetti et al., Nat. Mat. 15, 164 (2015). [2] L. Gragnaniello et al., Nano Lett. 17, 7177 (2017). [3] F. Paschke et al., 2018, submitted.

MA 28.5 Wed 10:30 H52

Four-dimensional inelastic neutron scattering intensity of cluster spin waves in ferromagnetic molecules — •Krunoslav Prsa and Oliver Waldmann — Physikalisches Institut, Universität Freiburg, Germany

The spin-wave approximation of many-body effects in magnetic solids can be adapted to describe excitations from the ferromagnetic ($S = S_{max}$) ground state in molecular nanomagnets. Starting from the Heisenberg Hamiltonian, this method provides exact solutions of the transitions from the ground state into the $M = M_{max} - 1$ sector, which are observed in inelastic neutron scattering (INS) experiments at low temperatures. We provide the analytical results for the INS intensity for isotropic and Ising anisotropic cases in powder and single crystal samples. We find that the complete $\vec{Q}$-dependence of intensity can be expanded in terms of few geometrical basis functions. A key consequence is that one can determine the eigenvectors directly from INS data, without the necessity to solve the magnetic model.

MA 28.6 Wed 10:45 H52

Element specific determination of the magnetic properties of the macrocyclic tetranucluer 3d-4f complexes with Cu3Tb core by means of x-ray magnetic circular dichroism (XMCD) — •K. Kuepper[1], K. Balinski[1], L. Schneider[1], J. Wöllermann[1], A. Buling[1], L. Joly[2], C. Piamonteze[3], H.L.C. Feltham[4], S. Brooker[4], A.K. Powell[5], and B. Delley[3] — [1]Fachbereich Physik , Universität Osnabrück, Barbarastr. 7, Osnabrück D-49069, Germany — [2]Universite de Strasbourg, CNRS, IPCMS, UMR 7504, Strasbourg F-67000, France — [3]Paul Scherrer Institute, Villigen CH-5232, Switzerland — [4]Department of Chemistry and the MacDiarmid Institute, University of Otago, P.O. Box 56, Dunedin 9054, New Zealand — [5]Institut für Anorganische Chemie, Karlsruhe Institute of Technology, Engesserstrasse 15, Karlsruhe D-76131, Germany

Feltham et al. synthesized molecules with Cu3Tb core using organic macrocyclic ligands, i.e. the propylene macrocycle (nickname: Cu3Tb(LPr)), which exhibits slow relaxation of magnetization [1], as well as a larger, butylene linked, macrocycle (nickname: Cu3Tb(LBu)) [2]. We used element specific XMCD to study the magnetic properties of these two molecules in external magnetic fields up to B=13.5 T and at temperatures between T=3K and T=10K [3]. We perform a sum rule analysis abd record element specific magnetization loops indicating a low value for the 3d-4f coupling. [1] H.L.C. Feltham et al., Inorg. Chem. 50, 4232 (2011). [2] H.L.C. Feltham et al., Inorg. Chem. 52, 3236 (2013). [3] K. Balinski et al., PCCP 20, 21286 (2018).

MA 28.7 Wed 11:00 H52

Inelastic Neutron Scattering Studies on a Family of 3*d*-4*f* Heterometallic Mn_2Ln_2 Single-Molecule Magnets — •Julius Mutschler[1], Krunoslav Prša[1], Christopher E. Anson[2], Annie K. Powell[2], and Oliver Waldmann[1] — [1]Physikalisches Institut, Universität Freiburg, Germany — [2]Institut für anorganische Chemie, Universität Karlsruhe, KIT, Germany

The discovery of slow relaxation and quantum tunneling of the magnetization in the now so-called single molecule magnets (SMMs) two decades ago has inspired both physicists and chemists alike. This class of molecules has been expanded to heterometallic clusters incorporating transition metal and rare earth ions. The 4*f* ions were chosen

because of their large angular momentum and magnetic anisotropy. Inelastic neutron scattering experiments were performed on the time-of-flight disk-chopper spectrometer IN6 at ILL on the SMM-series Mn_2Ln_2-squares with Ln=Y, Tb, Ho, Dy. Excellent data have been recorded, also for the Dy variety. The analysis of the data using a linked fit approach is presented.

MA 28.8 Wed 11:15 H52

Combining translational and spin-rotational symmetry in exact diagonalization of spin rings — •Tjark Heitmann[1] and Jürgen Schnack[2] — [1]Fachbereich für Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück — [2]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld

Exact diagonalization and other numerical studies of quantum spin systems are notoriously limited by the exponential growth of the Hilbert space dimension with system size. A common and well-known practice to reduce this increasing computational effort is to take advantage of the translational symmetry C_N in periodic systems. This represents a rather simple yet elegant application of the group theoretical symmetry projection operator technique. For isotropic exchange interactions, the spin-rotational symmetry $SU(2)$ can be used, where the Hamiltonian matrix is block-structured according to the total spin and magnetization quantum numbers. Rewriting the Heisenberg Hamiltonian in terms of irreducible tensor operators allows for an efficient and highly parallelizable implementation to calculate its matrix elements recursively in the spin-coupling basis. When combining both C_N and $SU(2)$, mathematically, the symmetry projection technique leads to ready-to-use formulas. However, the evaluation of these formulas is very demanding in both computation time and memory consumption – problems which are said to outweigh the benefits of the symmetry reduced matrix shape. We show a way to minimize the computational effort for selected systems and present the largest numerically accessible cases.