

O 13: Focus Session: New Trends in Molecular Magnetism (MA jointly with O, TT)

Organizers: J. Schnack (U. Bielefeld), O. Waldmann (U. Freiburg)

During the past 25 years molecular magnetism has developed into a broad field. Today's major research directions include applications in quantum computing or as quantum simulators as well as the use as sub-Kelvin magnetic refrigerants. For direct manipulation as part of spintronic systems molecules are deposited and manipulated on surfaces. The progress of this interdisciplinary field is intimately related to the ability of coordination chemists to synthesize unprecedented molecules, to the ability of experimental physicists to characterize them as well as to the ability of theorists to model their properties.

Time: Monday 15:00–17:30

Location: HSZ 04

Topical Talk O 13.1 Mon 15:00 HSZ 04
Spin dynamics in Molecular Nanomagnets — ●STEFANO CARRETTA — Dipartimento di Fisica e Scienze della Terra, Università di Parma, I-43124 Parma, Italy

Molecular nanomagnets (MNM) have been test beds for addressing several quantum phenomena. In particular, one of the major current objectives is to exploit their coherent spin dynamics for quantum information processing (QIP). We show that recently developed instrumentation yields the four-dimensional inelastic-neutron scattering function and enables the direct determination of the spin dynamics [1]. We use the Cr8 antiferromagnetic ring as a benchmark to demonstrate the potential of this approach, which allows us, for instance, to examine how quantum fluctuations propagate along the ring. We show that parameters of the spin Hamiltonian can be reliably calculated ab-initio. In particular, we present a flexible and effective ab-initio scheme to build many-body models for MNMs, and to calculate magnetic exchange couplings and zero-field splittings [2]. We have applied this scheme to three paradigmatic systems, the antiferromagnetic rings Cr8 and Cr7Ni and the single molecule magnet Fe4 and have found excellent agreement with experimental results. At last, we discuss the dynamics of ensembles of spin systems coherently coupled to microwave photons in coplanar waveguide resonators. We introduce a scheme to perform QIP that is based on a hybrid spin-photon qubit encoding [3].

[1] M. Baker et al, *Nature Physics* 8, 906 (2012); [2] A. Chiesa et al, *Phys. Rev. Lett.* 110, 157204 (2013); [3] S. Carretta, et al, *Phys. Rev. Lett.* 111, 110501 (2013).

Topical Talk O 13.2 Mon 15:30 HSZ 04
Exchange interaction in lanthanides — ●LIVIU CHIBOTARU, LIVIU UNGUR, NAOYA IWAHARA, and VEACESLAV VIERU — Theory of Nanomaterials Group, KU Leuven, Heverlee, Belgium

Using ab initio, DFT and model calculations we analyze the main features of exchange interactions in lanthanide complexes.

Andersons superexchange model is applied for analytical derivation of exchange interaction between total magnetic moments \mathbf{J}_1 and \mathbf{J}_2 corresponding to ground atomic multiplets of two exchange-coupled lanthanide ions. Despite the common belief that the exchange interaction is of $\sim \mathbf{J}_1 \cdot \mathbf{J}_2$ form, we find it strongly anisotropic. If the crystal field (CF) on Ln sites exceeds significantly the exchange splitting, the exchange interaction between low-lying CF doublet states generally becomes of non-collinear Ising type.

In the case of exchange-coupled lanthanide ion (\mathbf{J}) and isotropic magnetic center (\mathbf{S}) the exchange interaction is found not to be of the form $\sim \mathbf{J} \cdot \mathbf{S}$, as supposed before, but again very anisotropic. When the CF splitting on Ln exceeds the exchange splitting, the exchange interaction between the low-lying CF doublet on Ln and the isotropic spin generally becomes of collinear Ising type.

Finally, we give arguments why the mixed Ln-TM complexes are more efficient SMMs than pure Ln ones despite less anisotropic magnetic ions involved.

Topical Talk O 13.3 Mon 16:00 HSZ 04
Cool molecules — ●MARCO EVANGELISTI — Instituto de Ciencia de Materiales de Aragón, CSIC - Universidad de Zaragoza, Departamento

de Física de la Materia Condensada, 50009 Zaragoza, Spain

The recent progress in molecule-based magnetic materials exhibiting a large magnetocaloric effect at liquid-helium temperatures is reviewed. Advanced applications and future perspectives in cryogenic magnetic refrigeration are also discussed.

Topical Talk O 13.4 Mon 16:30 HSZ 04
Bulk and submonolayer studies of novel single-ion molecular magnets — ●JAN DREISER — Ecole Polytechnique Federale de Lausanne, Institute of Condensed Matter Physics, 1015 Lausanne, Switzerland — Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Single-ion magnets (SIMs) [1,2] contain a single transition-metal or rare-earth ion embedded in an organic ligand. In contrast to many other mononuclear molecular magnets, SIMs exhibit long magnetization relaxation times at low temperatures ranging from milliseconds to more than hours. In order to exploit their properties in possible applications they should be organized and addressable one-by-one [3]. A promising path to achieve this goal is the deposition of submonolayers of SIMs on to surfaces.

In this talk I will report on our recent studies of the Er(trensal) SIM [2] in which the Er(III) ion is seven-fold coordinated to the very robust tripodal ligand. In addition to the investigations of the bulk phase I will present first results obtained on (sub)monolayer deposits on metallic surfaces using X-ray magnetic circular dichroism and scanning tunneling microscopy.

[1] N. Ishikawa, M. Sugita, T. Ishikawa, S.-y. Koshihara, Y. Kaizu, *J. Am. Chem. Soc.* 2003, 125, 8694; [2] K. S. Pedersen, L. Ungur, M. Sigrist, A. Sundt, M. Schau-Magnussen, V. Vieru, H. Mutka, S. Rols, H. Weihe, O. Waldmann, L. F. Chibotaru, J. Bendix, J. Dreiser, submitted; [3] D. Gatteschi, A. Cornia, M. Mannini, R. Sessoli, *Inorg. Chem.* 2009, 48, 3408.

Topical Talk O 13.5 Mon 17:00 HSZ 04
When Organic Materials Interact with Ferromagnetic Surfaces: A First-Principles Perspective — ●NICOLAE ATODIRESEI — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The adsorption of π -conjugated organic materials on ferromagnetic surfaces offers the possibility to merge the concepts of molecular electronics with spintronics to build future nanoscale data storage, sensing and computing multifunctional devices. Based on the density functional theory, we performed theoretical studies to understand how to tailor the magnetic properties of organic-ferromagnetic interfaces. For such hybrid systems, the magnetic properties like molecular magnetic moments and their spatial orientation, the spin-polarization and the magnetic exchange coupling can be specifically tuned by an appropriate choice of the organic material and ferromagnetic surface. [1] N. Atodiresei et al., *Phys. Rev. Lett.* 105, 066601 (2010); [2] N. Atodiresei et al., *Phys. Rev. B* 84, 172402 (2011); [3] K. V. Raman et al., *Nature* 493, 509 (2013); [4] M. Callsen et al., *Phys. Rev. Lett.* 111, 106805 (2013).