MA 10 FV-internes Symposium "Molecular Magnetism" (Organizer: H.J. Krüger)

Zeit: Samstag 09:00–12:30 Raum: TU H1012

Hauptvortrag MA 10.1 Sa 09:00 TU H1012

The Molecular Approach to Nanomagnetism — •Roberta Sessoli — Department of Chemistry - INSTM, University of Florence, Italy

The observation about 10 years ago of magnetic bistability in molecules comprising a small number of interacting paramagnetic centers have renewed the interest in molecular magnetism. Molecules of this kind, also known as Single Molecule Magnets, have proven to be the ideal systems to investigate quantum effects in the dynamics of the macroscopic magnetization, like the tunnelling effect or the topological interference of tunnelling pathways. The research in the area is still very active and the emerging trends in the field will be the topics of this presentation.

Many efforts are actually devoted to the control of the organization of these molecules, for instance through the preparation of self-assembled monolayers on metallic surfaces. The objectives are the magnetic addressing and investigation of the single molecule as well as the investigation of the environmental effects, that are known to play a crucial role in the quantum dynamics of these objects.

Despite important achievements in the synthesis of new molecules, the blocking temperature, below which bistability is observed, remains quite low. Interestingly a sensible increase has been observed in molecular systems where anisotropic magnetic centers are arranged in 1d structures. These systems can be seen as the molecular analogues of monoatomic nanowires recently investigated.

Hauptvortrag MA 10.2 Sa 09:30 TU H1012

Minimum single-molecule magnets — •P. Müller[1], H. Rupp[1], R.W. Saalfrank[2], and M. Ruben[3] — [1]Physikalisches Institut III, Universität Erlangen-Nürnberg — [2]Institut für Organische Chemie, Universität Erlangen-Nürnberg — [3]Institut für Nanotechnologie, FZ Karlsruhe

Even without long-range magnetic order, some molecular crystals show hysteretic magnetization curves at low temperatures. This effect is a single-molecule property caused by a large uniaxial anisotropy combined with a high-spin ground state. This phenomenon has been observed in a class of cluster molecules containing Fe or Mn ions, with Mn_{12} acetate as a prototype. Until now, the effect is limited to temperatures below 4.2 K. In order to provide strategies for optimizing new systems, it is natural to focus on systems with a small number of metal ions. We present measurements on ferric stars $\mathrm{FeFe}_3\mathrm{L}_6$, where the star-like coupling topology forces a high-spin ground state of the molecule. We conclude our talk with recent results on mononuclear lanthanide-phthalocyanine double-decker molecules, which are promising candidates for higher working temperatures.

Hauptvortrag MA 10.3 Sa 10:00 TU H1012

Frustration effects in magnetic molecules — •Jürgen Schnack — Universität Osnabrück, Fachbereich Physik, D-49069 Osnabrück, Germany

Besides being a fascinating class of new materials, magnetic molecules provide the opportunity to study concepts of condensed matter physics in zero dimensions. This contribution will exemplify the impact of molecular magnetism on concepts of frustrated spin systems [1].

We will discuss spin rings and the unexpected rules that govern their low-energy behaviour. Rotational bands, which are experimentally observed in various molecular magnets, provide a useful, simplified framework for characterizing the energy spectrum, but there are also deviations thereof with far-reaching consequences. It will be explained in this context what localized independent magnons are and how they lead to giant magnetization jumps, a new macroscopic quantum effect [2]. In addition, frustration-induced plateaus of the magnetization and related susceptibility minima can be observed in magnetic molecules [3] as well as metamagnetic transitions. Finally, it is demonstrated that magnetic molecules could give rise to an enhanced magnetocaloric effect.

[1] J. Schnack, *Molecular Magnetism*, in *Quantum Magnetism*, Lecture Notes in Physics **645**, Springer, Berlin, Heidelberg (2004) 155-194
[2] J. Schulenburg, A. Honecker, J. Schnack, J. Richter, H.-J. Schmidt, *Macroscopic magnetization jumps due to independent magnons in frustrated quantum spin lattices*, Phys. Rev. Lett. **88** (2002) 167207
[3] C. Schröder *et al.*, *Competing Spin Phases in Geometrically Frustrated Magnetic Molecules*, Phys. Rev. Lett., submitted

Hauptvortrag MA 10.4 Sa 10:30 TU H1012

Frequency Domain Magnetic Resonance Spectroscopy on Molecular Magnets — •Joris van Slageren[1], Nadeschda Kirchner[1], Suriyakan Vongtragool[1], Marc Duran[1], Fadi El Hallak[1], Alexander Mukhin[2], Boris Gorshunov[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart — [2]General Physics Institute, Russian Academy of Sciences, Moscow, Russia

One of the most important parameters determining the properties of molecular magnets is the magnetic anisotropy in the form of zero-field splitting of the ground spin state. This parameter determines the energy barrier and therefore the slow magnetization relaxation dynamics. We have shown over the past years that frequency domain magnetic resonance spectroscopy (FDMRS) is excellently suited to the determination of zero-field splittings. Among its merits are: the lack of necessity of an external magnetic field, and easy access to very large zero-field splittings. Several pertinent examples will be shown. The magnetic resonance lineshapes give information on distributions in the sample as well as excited spin state dynamics. Because frequency and magnetic field are independent experimental parameters in the FDMRS technique, more sophisticated experiments can be performed. For example, we have spectroscopically studied the relaxation of the magnetization. We have demonstrated significant differences in line positions and line shapes between nonmagnetized and magnetized single molecule magnet samples. Finally, we will also show that single molecule magnets can function as tunable radiation polarization rotators in the THz range.

Hauptvortrag MA 10.5 Sa 11:00 TU H1012

Synthetic approaches to oxygen-bridged molecular magnets — •Annie Powell — Institut für Anorganische Chemie, Universität Karlsruhe, Engesserstr. 15, 76128 Karlsruhe

Hydrolysis reactions are a feature of the chemistry of many metal ions and usually lead to the formation of oxo- and hydroxo-bridged aggregates and then hydroxide, hydroxyoxide or oxide minerals. This chemistry can be controlled by supplying templating ligands which direct the size and shape of the intermediate aggregated species in a manner similar to that employed in Nature in biomineralisation processes. This makes it possible to favour the formation of molecular polymetal-oxo clusters which for paramagnetic metal ions have different magnetic properties from the related extended mineral phases as a result of the strong boundary effects operating in such systems. Furthermore, it is possible to functionalise the encapsulating ligands or supply linking synthons in order to enhance different types of supramolecular interactions amongst the molecules. This makes it possible to create 1-D chains, 2-D sheets or 3-D arrays of linked magnetic particles.

Hauptvortrag MA 10.6 Sa 11:30 TU H1012

Rational Design of Single-Molecule Magnets — •Thorsten Glaser — Institut für Anorganische und Analytische Chemie der Westfälischen Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 8, 48149 Münster

Single-molecule magnets are molecules that exhibit a magnetic bistability of pure molecular origin due to a slow relaxation of the magnetization. Thus, information can be stored in a single molecule with dimensions below 5 nm. The necessary prerequisites are a high spin ground state S along with a strong magnetic anisotropy of the easy-axes type which is described by a negative zero-field splitting D. We have started a program to obtain high spin ground states by ferromagnetic interactions between transition metal ions in polynuclear complexes. In order to control the coupling of the transition metal ions we perform a ligand design based on the principles of double exchange, orthogonality of the magnetic orbitals and spin-polarization. Magnetic anisotropy is introduced by enforcing a strong tetragonal ligand field on the transition metal ions. We have successfully synthesized two heptanuclear transition metal complexes with high spin ground states and magnetic anisotropy: Mn6Cr with $S = 21/2$ and Fe6Cr with $S = 27/2$. Their magnetic properties and single-molecule magnet behavior will be presented.

Hauptvortrag

MA 10.7 Sa 12:00 TU H1012

Switchable Molecules — •Philipp Gütlich — Institut für Anorganische Chemie und Analytische Chemie, Universität Mainz, Staudingerweg 9, 55099 Mainz, Germany

Coordination compounds of transition metal ions with open-shell electron configurations may exhibit dynamic electronic structure phenomena, depending on the nature of the coordinating ligand sphere. Thermal, light- and pressure-induced changes of spin states [1-3] are among the most fascinating electronic games encountered in molecular magnetism of transition metal compounds, which are presently under extensive study by chemists and physicists. The switching properties make such material potential candidates for practical applications in thermal and pressure sensors as well as optical devices. The basics of thermal and optical spin transition will be briefly reviewed. Selected examples of thermal spin crossover complexes will be discussed.It will be shown that switching forth and back between different spin states may be effected with light of different wave lengths. The effect of pressure on the spin transition behaviour will be demonstrated. Possible practical applications will be discussed.

[1] P. Gütlich, Y. Garcia, T. Woike: "Photoswitchable Coordination Compounds"Coord.Chem. Rev. 219-221 (2001) 839-879 [2] P. Gütlich, Y. Garcia, H. Spiering: "Spin Transition Phenomena", in: Magnetism: Molecules to Materials IV, J.S. Miller, M. Drillon (eds.), Wiley-VCH 2003 [3] P. Gütlich, H. A. Goodwin (eds.), "Spin Crossover in Transition Metal Compounds", Topics in Current Chemistry, volumes 233, 234, 235, Springer 2004, Berlin-Heidelberg-New York.