

## TT 17 Symposium Quantum Magnetism in Molecule-based Materials

Zeit: Montag 10:15–13:00

Raum: TU H104

**Hauptvortrag**

TT 17.1 Mo 10:15 TU H104

**From Spin to Quantum Order in Coordination Polymer Magnets** — ●COLLIN BROHOLM — Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218, USA

Coordination polymer magnets feature transition metals such as Cu and Ni on a range of different lattices and offer opportunities for exploring qualitatively different cooperative phases of quantum many body systems. This talk will present an overview of neutron scattering experiments that have been performed to understand spin dynamics in systems ranging from spin-chains (copper pyrazine dinitrate,  $\text{CuCl}_2 \cdot 2\text{dimethylsulfoxide}$ , NENP, and NDMAP) through a spin-ladder ( $\text{Cu}(\text{Quinoxaline})\text{Br}_2$ ) to frustrated two and three dimensional systems (PHCC and  $\text{CuHpCl}$ ). While the isolated spin-1/2 chain systems are quantum critical and can develop spin order due to weak inter-chain interactions at sufficiently low temperatures, cooperative singlet ground states are in fact more common in these low symmetry antiferromagnetic spin systems. The qualitatively different excitations spectra of gapless and gap-full systems will be described as well as their different responses to applied magnetic fields.

**Hauptvortrag**

TT 17.2 Mo 10:50 TU H104

**Design, Synthesis and Study of Model Quantum Magnets** — ●ANDREW HARRISON — School of Chemistry, The University of Edinburgh, Edinburgh, EH9 3JJ, UK

A major constraint on experimental studies of model magnets is the availability of suitable samples that provide tangible models to inspire or test theory. Some degree of rationalisation or even control may be introduced to synthetic strategies through consideration of bonding models: close-packing of spheres may be used to rationalise structures of ionic systems, while the linking of co-ordination polyhedra or vertices with a particular point group has some predictive power for systems where covalent bonding is prevalent. These strategies will be illustrated through the consideration of model frustrated systems such as triangular and kagome lattices, and specific examples will be given of model systems with  $S = \frac{1}{2}$  on such lattices, one of which shows evidence for a quantum ground state. We will also consider the possibility of tuning systems strongly through accessible magnetic fields and diamagnetic doping to access quantum phases. What is required here are low-spin, low-dimensional (and perhaps also frustrated) antiferromagnets with relatively weak magnetic exchange and diamagnetic analogues that either isostructural, or close to being so. Examples of copper salts that act as model  $S = \frac{1}{2}$  square Heisenberg antiferromagnets are presented

**Fachvortrag**

TT 17.3 Mo 11:30 TU H104

**Molecular solids - model systems for exploring quantum magnetism in reduced dimensions** — ●MICHAEL LANG<sup>1</sup>, BERNHARD BRENDEL<sup>1</sup>, ANDREAS BRÜHL<sup>1</sup>, JÖRG MAGERKURTH<sup>1</sup>, VOLODYMYR PASHCHENKO<sup>1</sup>, BERND WOLF<sup>1</sup>, LARISA ZHERLITSINA<sup>2</sup>, NORBERT AUNER<sup>2</sup>, GÜNTER MARGRAF<sup>2</sup>, HANS LERNER<sup>2</sup>, and MATTHIAS WAGNER<sup>2</sup> — <sup>1</sup>Physikalisches Institut, J.W. Goethe-Universität Frankfurt, FOR 412, 60054 Frankfurt — <sup>2</sup>Institut für Anorganische Chemie, J.W. Goethe-Universität, Frankfurt, FOR 412, 60439 Frankfurt

By combining open-shell transition metal ions with suitable organic linkers flexible building block systems may be produced for generating novel classes of materials, especially quantum magnets with distinct exchange-coupling topologies. A particularly interesting feature of these molecule-based magnets is their small exchange coupling constants  $J$ , weak enough for laboratory magnets to drive the systems into the interesting high-field regime where  $g\mu_B B > J$ . In this contribution we will discuss various realizations of molecule-based low-dimensional quantum magnets such as  $\text{Cu}(\text{II})$  cyclosiloxanolate complexes or a  $\text{Cu}(\text{II})$  coordination polymer. The latter system can be used to study generic magnetocaloric and magnetoelastic properties of the antiferromagnetic  $S = 1/2$  Heisenberg chain near the saturation field.

**Fachvortrag**

TT 17.4 Mo 12:00 TU H104

**Magnetocaloric effect in frustrated and molecular magnets** — ●ANDREAS HONECKER — Technische Universität Braunschweig, Institut für Theoretische Physik, 38106 Braunschweig, Germany

Due to the magnetocaloric effect, adiabatic changes of the field applied

to a magnet yield a change of temperature. Adiabatic demagnetization of a paramagnetic salt was the first method to achieve temperatures below 1K. Recently, there has been renewed interest in cooling by adiabatic demagnetization for room-temperature applications. Also low-temperature records are still established by this method.

We discuss recent theoretical results for the magnetocaloric effect in the vicinity of field-induced quantum phase transitions in correlated and molecular magnets. Geometrically frustrated magnets are of special interest since they exhibit large entropies at low temperatures, promising a large magnetocaloric effect. In particular a comparative study of different one-dimensional quantum magnets shows that lower temperatures can indeed be achieved by adiabatic (de)magnetization of a frustrated system as compared to a non-frustrated one. Finally, we discuss potential applications of frustrated quantum magnets for efficient low-temperature magnetic refrigeration.

TT 17.5 Mo 12:30 TU H104

**Quantum sine-Gordon behaviour in copper pyrimidine dinitrate** — ●R. FEYERHERM<sup>1</sup>, S. A. ZVYAGIN<sup>2</sup>, and A. U. B. WOLTER<sup>3</sup> — <sup>1</sup>Hahn-Meitner-Institut, 14109 Berlin, Germany — <sup>2</sup>NHFL, Florida State University, Tallahassee, FL 32310, U.S.A. — <sup>3</sup>IMNF, TU Braunschweig, 38106 Braunschweig, Germany

Copper pyrimidine dinitrate has been recently identified as  $S = 1/2$  antiferromagnetic chain with a field-induced spin gap [1], and turned out to be one of the best realizations of the quantum sine-Gordon spin chain model known to date. The field-induced gap arises from a perturbation from the isotropic Heisenberg chain by an alternating  $g$ -tensor and the Dzyaloshinskii-Moriya (DM) interaction. Other consequences of this perturbation are an intrinsic Curie-like contribution to the magnetic susceptibility [1], a large field-induced staggered magnetization perpendicular to the applied field [2], and a  $T^{-2}$  contribution to the ESR-linewidth [3]. Most interestingly, in recent high-field submillimeter wave ESR studies of the gapped state signatures of three breather branches and a soliton, besides several multi-particle excitations, have been identified and allowed for a detailed comparison with predictions from the quantum-sine Gordon field theory [4].

- [1] R Feyerherm *et. al.*, J. Phys.: Condens. Matter. 39 (2000) 8495
- [2] A.U.B. Wolter *et. al.*, Phys. Rev. B 68 (2003) 220406(R)
- [3] T. Asaono *et. al.*, Physica B 329-333 (2003) 1006
- [4] S. A. Zvyagin *et. al.*, Phys. Rev. Lett. 93 (2004) 027201

TT 17.6 Mo 12:45 TU H104

**Magnetic properties of a molecular based antiferromagnet on a honeycomb lattice** — ●IVAN SPREMO and PETER KOPIETZ — Institut für Theoretische Physik, Universität Frankfurt, Robert-Mayer-Str. 8, 60054 Frankfurt am Main

Using a modified spin-wave approach and exact diagonalizations we have calculated the finite-temperature magnetization curve  $M(H)$  of a two-dimensional quantum Heisenberg antiferromagnet on a honeycomb-lattice in a uniform magnetic field  $H$ . Our theoretical curve for  $M(H)$  agrees reasonably well with recent experimental data obtained for a molecular based antiferromagnet with stoichiometric formula  $\text{C}_{22}\text{H}_{18}\text{MnO}_8$ . We also discuss the nature of the spin-excitations of quantum antiferromagnets in a uniform magnetic field at zero temperature. We show that below three dimensions the coupling between transverse and longitudinal spin fluctuations leads to a breakdown of the quasi-particle concept for magnons.