

et al., Angew. Chem. Int. Ed. Engl. 39 (2000) 1612.

MA 27.7 Thu 16:00 EB 202

Broadband electron paramagnetic resonance of single-molecule magnets at millikelvin temperatures. — ●KONSTANTIN PETUKHOV¹, KLAUS GIEB¹, THORSTEN GLASER², WOLFGANG HANSEN³, and PAUL MÜLLER¹ — ¹Institut für Physik der Kondensierten Materie, Universität Erlangen-Nürnberg — ²Lehrstuhl für Anorganische Chemie I, Universität Bielefeld — ³Institut für Angewandte Physik, Universität Hamburg

We present a technique which combines Hall-bar magnetometry of single-molecule magnets (SMMs) with broadband microwave absorption measurements. This electron paramagnetic resonance-like spectroscopy can be performed at millikelvin temperatures and enables the use of short-pulsed microwave radiation. Thus, the spin dynamics of SMMs can be studied. We present measurements on novel Mn₆Mn and Mn₆Cr single-molecule magnets.

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Spin-dynamics of ferric wheels in high magnetic fields — ●LARS SCHNELZER and BERND PILAWA — Physikalisches Institut, Universität Karlsruhe (TH), D-76131 Karlsruhe

The dynamic properties of the antiferromagnetic cyclic hexanuclear iron(III) complexes ²³Na/⁷Li@Fe₆(tea)₆ have been studied by means of nuclear magnetic resonance. We analyzed the longitudinal relaxation rate T_1^{-1} of the central alkali ions ²³Na and ⁷Li in the magnetic field range up to 20 T at a temperature of 2 K. The T_1^{-1} measurements reveal the influence of the levelcrossing between the S=0 and S=1 states by an enhanced relaxation rate, as well as a strong decrease of the relaxation rate at characteristic fields between level crossings. In comparison with the calculated fluctuation spectrum of the electronic spins this suppression of the T_1 -rate indicates an extremely reduced line width of the electronic resonance around $\omega=0$ (the so called ω_0 -resonance).

MA 27.9 Thu 16:30 EB 202

Coordination geometry induced changes on magnetic parameters of Cu(II) complexes — ●BJÖRN BRÄUER¹, TOBIAS RÜFFER¹, DANTE GATTESCHI², MARIA FITTIPALDI², ANDREA CANESCHI², FLORIAN WEIGEND³, and GEORGETA SALVAN¹ — ¹Chemnitz University of Technology, Department of Physics, Reichenhainer Straße 70, D-09126 Chemnitz — ²University of Florence, Department of Chemistry, Via della Lastruccia 3, I-50019 Florence — ³Forschungszentrum Karlsruhe, Institute for Nanotechnology, Postfach 3640, D-76021 Karlsruhe

Cu(II)-bis(oxamato) complexes are prominent representatives for basic research studies of magnetic exchange phenomena [1]. We have used Electron Paramagnetic Resonance (EPR) spectroscopy to study the dependence of the hyperfine coupling constants A and the spin density distribution on the structural parameters of mono-nuclear complexes. Furthermore, the influence of such variations on the super exchange coupling parameter J of the respective tri-nuclear complexes was investigated. It was shown that deviations from the square planar coordination geometry decrease the delocalisation of spins leading to a smaller J value, i. e. a smaller antiferromagnetic interaction. The obtained parameters were also calculated by means of Density Functional Theory (DFT). The J parameters were determined using the broken symmetry approach and the influence of packing effects, counter ions, and bridging ligands were investigated. The CONductor like Screening Field MOdel (COSMO) was found to be a suitable model for reliable predictions of experimental trends. [1] O. Kahn, Molecular Magnetism, VCH Weinheim, 1993.

MA 27.10 Thu 16:45 EB 202

Enhanced magnetocaloric effect in frustrated magnetic molecules with icosahedral symmetry — ●JÜRGEN SCHNACK¹ and JOHANNES RICHTER² — ¹Universität Bielefeld, Fakultät für Physik, PF 100131, D-33501 Bielefeld — ²Universität Magdeburg, Institut für Theoretische Physik, PF 4120, D-39016 Magdeburg

We investigate the magnetocaloric properties of certain antiferromagnetic spin systems that have already been or very likely can be synthesized as magnetic molecules. It turns out that the special geometric frustration which is present in antiferromagnets that consist of corner-sharing triangles leads to an enhanced magnetocaloric effect with high cooling rates in the vicinity of the saturation field. These findings are compared with the behavior of a simple unfrustrated spin ring as well as with the properties of the icosahedron. To our surprise, also for the

icosahedron large cooling rates can be achieved but due to a different kind of geometric frustration. [J. Schnack, R. Schmidt, J. Richter, Phys. Rev. B **76** (2007) 054413]

MA 27.11 Thu 17:00 EB 202

Electronic structure of phthalocyanines — ●PREDRAG LAZIC, NICOLAE ATODIRESEI, and STEFAN BLÜGEL — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

The coupling between the π -delocalized electrons of the phthalocyanine with the d -localized electrons of a metal yields to a class of organometallic molecules with interesting physical properties. We have performed the *ab-initio* calculations on the gas phase of metal-phthalocyanine molecules as well as their adsorption on a Cu(111) surface precovered with a monolayer of sodium chloride. In order to describe accurately the molecule-substrate interaction we have used the seamless approach to include the long range correlation effects (i.e. van der Waals interaction) which are not properly described in the present DFT codes using LDA or GGA exchange-correlation functionals.

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Approximate spectra for magnetic molecules with sublattice structure — ●ROMAN SCHNALLE¹ and JÜRGEN SCHNACK² — ¹Universität Osnabrück, Fachbereich Physik, D-49069 Osnabrück — ²Universität Bielefeld, Fakultät für Physik, PF 100131, D-33501 Bielefeld

A lot of interesting magnetic molecules cannot be treated with numerically exact diagonalization routines because of the huge dimensions of the Hilbert spaces. Therefore approximate numerical techniques are highly desirable to obtain information about the energy spectra of the investigated systems. In a recent work we developed a perturbation theory that is guided by an approximate Hamiltonian for spin systems with sublattice structure, the rotational band Hamiltonian [1]. Within this perturbative approach an increasing number of states is taken into account. These states are chosen to be those with low-lying energies in the spectrum of the rotational band Hamiltonian [2].

[1] J. Schnack, M. Luban, Phys. Rev. B **63**, 014418 (2000)

[2] O. Waldmann, Phys. Rev. B **75**, 012415 (2007)

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Electronic and Magnetic Properties of Mn₁₂ Single-Molecule Magnets on the Au(111) Surface — ●SÖNKE VOSS¹, MICHAEL BURGERT¹, MIKHAIL FONIN¹, CHRISTIAN MICHAELIS², IVAN BRIHUEGA², YURY S. DEDKOV³, ULRICH GROTH¹, KLAUS KERN², and ULRICH RÜDIGER¹ — ¹Universität Konstanz, 78457 Konstanz — ²Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart — ³Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden

The paramount interest in single-molecule magnets (SMMs) like Mn₁₂-acetate and its derivatives was inspired by numerous experimental and theoretical insights indicating the feasibility of addressing quantum effects of magnetism on a molecular scale. Due to its relatively high blocking temperature (~3K) combined with the ability to identify well-defined spin states, Mn₁₂ still remains the most favoured SMM possibly allowing the detection of magnetic fingerprints in transport properties of a single molecule.

In this work, the electronic properties of Mn₁₂ molecules chemically grafted on Au(111) surfaces have been studied by means of low temperature as well as room temperature scanning tunneling microscopy and spectroscopy (STS), x-ray absorption spectroscopy and photoelectron spectroscopy. The results revealed signatures from most probably intact Mn₁₂ molecules while STS measurements in magnetic fields indicate the possibility to identify magnetic fingerprints in scanning tunneling spectra. The results will be discussed with respect to previous attempts to perform transport measurements on Mn₁₂ SMMs.

MA 27.14 Thu 17:45 EB 202

Fe-porphyrin monolayers on ferromagnetic substrates: Electronic structure and magnetic coupling strength — ●MATTHIAS BERNIEN¹, XIAOYING XU¹, JORGE MIGUEL¹, MARTEN PIANTEK¹, PHILIPP ECKHOLD¹, JUN LUO¹, JULIA KURDE¹, KLAUS BABERSCHKE¹, WOLFGANG KUCH¹, HEIKO WENDE², and PANKAJ SRIVASTAVA² — ¹Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — ²Fachbereich Physik, Experimentalphysik - AG Wende, Universität Duisburg-Essen, Lotharstrasse 1, D-47048 Duisburg, Germany