

MA 37 Molecular Magnetism

Time: Friday 10:45–13:15

Room: HSZ 403

MA 37.1 Fri 10:45 HSZ 403

Exploring molecular magnetism by first-principles density-functional-theory calculations — ●JENS KORTUS — Theoretische Physik, TU Bergakademie Freiberg

Magnetism at the molecular scale holds great promises for future applications in information storage. However, before any applications we have to understand the relevant processes which are governed by the laws of quantum mechanics in detail. The magnetic properties at this length scale are determined by exchange interactions and spin-orbit interaction. The exchange interaction will determine the magnetic ground state of the molecule. The spin-orbit coupling is responsible for the magnetic anisotropy, which is one of the key properties of a single molecule magnet. First-principles density functional theory (DFT) calculations offer an insight in the electronic structure and molecular orbitals and allows for the calculation of exchange interaction and spin-orbit coupling.

We will compare our theoretical results to experimental ones for magnetic anisotropies. For many systems the agreement is very good, however there are also cases where DFT underestimates the magnetic anisotropy by a factor of two. Other possible application of DFT to molecular systems include the calculation of STM spectra, which can be directly compared to experiment allowing for a check of the calculated charge densities.

MA 37.2 Fri 11:00 HSZ 403

Frequency Domain Magnetic Resonance Spectroscopy in Molecular Magnetism — ●JORIS VAN SLAGEREN — 1. Physikalisches Institut, Universität Stuttgart

In recent years, we have developed an advanced magnetic resonance technique called frequency-domain magnetic resonance spectroscopy (FDMRS) and applied it to the study of a number of phenomena in molecular magnetism. We are interested in the magnetic anisotropy of molecular magnets especially in the form of zero-field splitting of the ground state multiplet. We have shown that FDMRS is a very efficient and accurate method to determine the parameters that describe the magnetic anisotropy. Our aim is to understand the physical origin of the zero-field splitting in exchange coupled clusters, and the role played by the single ion anisotropy and the mixing of spin multiplets. In addition, we have become interested in the (especially dipolar) interaction between single molecule magnets in the crystal and its influence on the magnetic relaxation. To this end we have studied the magnetic resonance line-shape in frozen solutions of single-molecule magnets. Our ability to vary frequency and field independently allows us to perform more sophisticated experiments. For example, we have shown that we can investigate quantum tunneling of the magnetization. Finally we have shown that single molecule magnets can function as efficient Faraday rotators of the radiation polarization in the terahertz frequency range.

MA 37.3 Fri 11:15 HSZ 403

A ^{23}Na -NMR study of the ferric wheel system $\text{Na@Fe}_6(\text{tea})_6$ — ●LARS SCHNELZER, ROLAND LEPPIN, and BERND PILAWA — Physikalisches Institut, Universität Karlsruhe (TH), D-76131 Karlsruhe

The hexanuclear iron(III) complex $\text{Na@Fe}_6(\text{tea})_6$ consists of a ring of six Fe(III) ions which are coupled by organic ligands and centered by a ^{23}Na -alkali atom. The dynamic properties of $\text{Na@Fe}_6(\text{tea})_6$ have been studied by ^1H and ^{23}Na NMR measurements at 52 MHz. The temperature dependence of the ^1H T_1 rate reveals a peak at 30 K which is a characteristic feature of the ferric wheel systems whereas the ^{23}Na NMR T_1 rate measurements increase linearly with temperature indicating a purely quadrupolar relaxation of the nuclear spin. In order to study the influence of the electronic spin system on the NMR properties of the ^{23}Na nucleus, the magnetic field and temperature dependence of the T_1 rate has been measured on a polycrystalline sample. The field dependence shows the strong enhancement of the T_1 rate due to the level crossing between the $S=0$ groundstate and the first excited $S=1$ state in the field range between $B_{\parallel} \sim 11$ T and $B_{\perp} \sim 13$ T, proving the influence of the Fe(III) spin on the ^{23}Na nucleus. In contrast to the measurements at 52 MHz, the temperature dependence of T_1 at 79.5 MHz is characterized by a strong increase up to $T \sim 30$ K and a broad maximum, resembling the ^1H measurements of T_1^{-1} on the $\text{Fe}_6(\text{tea})_6$ system, when the magnetic field is oriented parallel to the molecular symmetry axis.

MA 37.4 Fri 11:30 HSZ 403

Magnetic Anisotropy Energies of Metal-Benzene Sandwiches — ●NICOLAE ATODIRESEI¹, YURIY MOKROUSOV², GUSTAV BIHLMAYER¹, and STEFAN BLÜGEL¹ — ¹Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany — ²Institute of Applied Physics and Microstructure Research Center, University of Hamburg, 20355 Hamburg, Germany

Molecular magnets moved to the frontier of research as ideal candidates for the smallest possible magnets. We performed *ab initio* calculations for one-dimensional (1D) magnetic organometallic sandwiches, $M_n Bz_m$ ($Bz = C_6H_6$; $M = V, Nb, Ta$) and infinite wires within the framework of the density functional theory (DFT) in the generalized gradient approximation (GGA) using the full-potential linearized augmented plane-wave method for 1D-systems [1,2]. We found that all the $M_n Bz_m$ molecules and the infinite wires are magnetic. By including the spin-orbit coupling in the total energy calculations we considered the two possible symmetry-determined directions of the magnetization in the molecules and wires: along the z-axis (z) and radial, parallel to the plane of the benzenes (r). The magnetic anisotropy energy (MAE) describes the energy difference between them. We conclude that by replacing the V atoms with heavier metals such as Nb and Ta, leads to a stronger spin-orbit interaction with larger MAE's. The $(NbBz)_{\infty}$ wire shows a ballistic anisotropic magnetoresistance (BAMR)[3] effect. [1] Y. Mokrousov et al. PRB 72 (2005); [2] <http://www.flapw.de>; [3] J. Velev et al. PRL 94 (2005)

MA 37.5 Fri 11:45 HSZ 403

Spin-dependent transport through half-metallic organometallic wires — ●V. MASLYUK¹, A. BAGRETS^{1,2}, T. BREDOW³, M. BRANDBYGE⁴, and I. MERTIG¹ — ¹Martin-Luther-Universität at Halle-Wittenberg, Fachbereich Physik, Germany — ²Institut für Nanotechnologie, Forschungszentrum Karlsruhe, Germany — ³Institut für Theoretische Chemie, Universität at Hannover, Germany — ⁴Department of Micro and Nanotechnology, Technical University of Denmark, Denmark

During the last years, molecular magnets have been attracting enormous attention, since they are candidates for future applications in high-density information storage and quantum computers. Here, we present a first class of magnetic one-dimensional organometallic systems which show half-metallic behaviour and can be synthesized [1]. These systems are $\text{Met-C}_6\text{H}_5\text{H}_2\text{C}_6\text{H}_5$ multi-decker clusters, with $\text{Met}=\text{V}, \text{Mn}$ and Co [2]. Theoretical investigations of the transport properties of such organometallic wires are presented. The conductance and the electronic structure of the molecular wires were calculated by means of a LCAO method based on density functional theory combined with non-equilibrium Greens functions [3]. A detailed analysis of electronic, magnetic and transport properties is given. A large spin-polarization of the electron current is predicted. Furthermore, the influence of the small molecules, H_2 , N_2 , O_2 and CO , on the transport properties of organometallic wires is discussed.

[1] K.Miyajima, *et al.*, Eur.Phys.J.D {bf 34},177(2005) [2] V.V.Maslyuk, *et al.*, [cond-mat/0510144]. [3] M.Brandbyge, *et al.*, PRB {bf 65}, 165401(2002).

MA 37.6 Fri 12:00 HSZ 403

Field-dependent magnetic parameters in $\{\text{Ni}_4\text{Mo}_{12}\}$ — ●MIRKO BRÜGER and JÜRGEN SCHNACK — Universität Osnabrück, Fachbereich Physik, Barbarastr. 7, D-49069 Osnabrück

$\text{Mo}_4\text{V}_2\text{O}_{30}(\mu_2 - \text{OH})_{10}\text{H}_2\{\text{Ni}^{\text{II}}(\text{H}_2\text{O})_3\}_4$ is a magnetic molecule which on first glance looks rather unspectacular since it comprises four Ni ions which are placed at the vertices of an almost ideal tetrahedron and connected by oxygen bridges. Thus one would expect that the magnetic energy levels are reasonably well described by an isotropic Heisenberg model with antiferromagnetic coupling. Preliminary experimental results, obtained by our experimental collaborators in Ames (USA) and Okayama (Japan), show a low-temperature magnetization curve (M vs. B) with increasing step size. The magnetization curve shows two equal steps at low fields and two larger steps of similar size at high fields, which are rounded off anisotropy. Even including biquadratic exchange and Dzyaloshinskii-Moriya interaction we were unable to describe the low-temperature magnetization curve. Furthermore low-field susceptibil-