MA 36: Magnetic Particles and Clusters II

Time: Thursday 15:15–18:15 Location: HSZ 401

MA 36.1 Thu 15:15 HSZ 401

Ligand-dependence of longterm stability of cobalt nanoparticles — •Britta Vogel, Axel Dreyer, Nadine Mill, Anna Regtmeier, Inga Ennen, Daniel Ebke, Simone Herth, and Andreas Hütten — Department of Physics, University of Bielefeld, D-33615 Bielefeld, Germany

Cobalt nanoparticles with a diameter of 12nm have initially been prepared with TOPO. Subsequently a ligand exchange was carried out so as to employ the ligand of choice to the nanoparticles. The effect of different ligands on the change of the magnetic moment of the particles was investigated systematically by using ligands with two different head groups, several different chain lengths with and without double bond, several numbers of chains and two ligands with benzene rings. The samples were stored at different temperatures to gain insight into the temperature dependence of the oxidation.

MA 36.2 Thu 15:30 HSZ 401

Imaging magnetic responses of different Fe nanocube configurations — •Nina Friedenberger[1], Katharina Ollefs[1], Florian Kronast[2], Hermann Dürr[2], and Michael Farle[1] — [1]Experimentalphysik-AG Farle, Fachbereich Physik, Universität Duisburg-Essen, Germany — [2]BESSY GmbH, Berlin, Germany

While structural properties of self-assembled particles can be studied using electron microscopy, a magnetic characterization is presently mostly based on ensemble averaging. Here we use high lateral resolution photoemission electron microscopy (PEEM) and x-ray magnetic circular dichroism (XMCD) spectroscopy to overcome this limitation. We studied Fe nanoparticles with a cubic shape [1] in the PEEM with a lateral resolution of typically 30nm. In order to identify the local coordination of the particles we matched the PEEM images to scanning electron microscopy (SEM) images of higher lateral resolution. PEEM images were taken in an applied magnetic field of up to +/- 33mT which allowed us to extract the hysteresis behavior of different configurations at temperatures down to 110K. Our results demonstrate that the magnetic properties of the investigated Fe nanoparticles depend strongly on their local coordination. Obviously strong magnetic dipolar coupling between neighboring particles influences their magnetic response. Financially supported by: DFG (SFB 445) and EC: MC-RTN "SyntOrbMag". [1] A. Shavel, et al. Adv. Funct. Mat. 17 (2007) 3870-3876

MA 36.3 Thu 15:45 HSZ 401

Micro Hall Magnetometry on individual iron filled carbon nanotubes — •Kamil Lipert[1], Franziska Wolny[1], Thomas Mühl[1], Pintu Das[2], Jens Müller[2], Rüdiger Klingeler[1], and Bernd Büchner[1] — [1]Leibniz-Institute for Solid State and Materials Research (IFW) Dresden — [2]Max Planck Institute for Chemical Physics of Solids (MPI-CPfS) Dresden

We present the fabrication and structural characterization of a gated (Al,Ga)As Micro- Hall device and its application for studying the magnetic properties of iron filled carbon nanotubes. The nanomagnets have been positioned in the center of the active area of 800*800nm^2 by means of a Scanning Electron Microscope (SEM) equipped with micromanipulators. The Hall-voltage was measured under applied magnetic fields up to 1T at temperatures 5K $\leq T \leq$ 90K in the ballistic regime. The z-component of the stray field of the nanomagnet has been extracted and the magnetisation reversal has been studied in detail. Interestingly, we found unusual multi-step hysteresis curves which can be tentatively explained by magnetic field induced bending of the free-standing carbon nanotube. This might open the possibility of practical application as for example a nano-switch.

MA 36.4 Thu 16:00 HSZ 401

Decoupling of the surface and core magnetic contribution in antiferromagnetic nanostructures — •Maria Jose Benitez[1,2], Oleg Petracic[1], Harun Tüysüz[2], Florin Radu[3], Ferdi Schüth[2], and Hartmut Zabel[1] — [1]Institut für Experimentalphysik/Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum — [2]Max-Planck Institut für Kohlenforschung, D-45470 Mülheim an der Ruhr — [3]BESSY GmbH, Albert-Einstein Strasse 15, D-12489 Berlin

Ferromagnetic particles enter superparamagnetism upon decreasing their size. However, antiferromagnetic nanoparticles are governed by core-shell behavior. We present a systematic magnetometry study on antiferromagnetic Co_3O_4 and CoO nanowires with various structure sizes between 5 and 10nm. We identify two different magnetic contributions, viz. one being governed by the antiferromagnetically ordered wire cores. The second one is attributed to the antiferromagnetic surface. We demonstrate that the surface behaves as a two-dimensional diluted antiferromagnet in a field (DAFF) [1]. Furthermore we show that measurements of the thermoremanent (TRM) and isothermoremanent magnetization (IRM) can serve as a magnetic fingerprint of particularly the surface contribution to the magnetization.

[1] M. J. Benitez et al., Phys. Rev. Lett. 101, 097206 (2008).

MA 36.5 Thu 16:15 HSZ 401

Surface energies of Fe, Co, Mn, Pt and their alloys: An *ab initio* study — •Antje Dannenberg, Markus Ernst Gruner, and Peter Enetl — Universität Duisburg-Essen, 47048 Duisburg, Germany

$L1_0$-ordered FePt and CoPt nanoparticles are considered as promising materials for ultra-high density magnetic recording applications. Since the energies of surfaces and internal interfaces play an important role in determining the equilibrium shape of the particles, their analysis is of fundamental interest.

We here show the results of a systematic study of the energies and magnetism of low-indexed surfaces for the monoatomic systems Fe, Co, and Pt, as well as for the binary alloys FePt, CoPt, and MnPt. For $L1_0$-ordered, stoichiometric alloys we present a method which is based on surface energy phase diagrams in order to evaluate the surface energy contributions of the single material components. For transition metals this has not been done before. We find, that especially platinum covered {111} facets show extraordinary low surface energy while the (001) surface, which is needed for the desired $L1_0$-cuboctahedron, lays higher in energy. This gives rise to the appearance of multiply twinned icosahedra in gas phase experiments. The energies are calculated within density functional theory using the VASP code and the surfaces were modeled within the slab approach.

MA 36.6 Thu 16:30 HSZ 401

Effect of Pt capping on the magnetic anisotropy of 3*d* clusters — •Sanjubala Sahoo[1], Peter Entel[1], and Manuel Richter[2] — [1]Physics Department, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]IFW Dresden e.V., D-01171 Dresden, Germany

Clusters show large magnetic anisotropy compared to bulk because of spatial confinement. The enhanced anisotropy in clusters is a favorable property explored by the data storage technologies, which aim to develop miniature devices. Systems like FePt alloys are active candidates for the same. We study the magnetic anisotropy of 13 atom icosahedral clusters of Fe, Co and Ni, respectively, using the density functional theory. In our studies, the anisotropy is treated by including the spin-orbit interaction in a scalar relativistic approximation in the density functional Hamiltonian. Our studies show that the spin and orbital moments of clusters are larger than that of bulk. The magnetic anisotropy is also enhanced as compared to the corresponding bulk values. The role of Pt in the magnetic anisotropy of clusters is studied by capping Fe cluster with Pt atoms. Capping such a 5*d* element on a 3*d* cluster is observed to change the cluster's anisotropy energy, which will be discussed in our contribution.

MA 36.7 Thu 16:45 HSZ 401

Antiferromagnetic finite nanowires: Heisenberg spin model revisited — •Mohammed Ahsanul Hoda Ahsan[1,2], Jamal Berakdar[1], and Mohammed Mahfoozul Haque[2] — [1]Institute of Physics, Martin-Luther University, Halle-Wittenberg, Heinrich-Damerow Str.-4, 06120 Halle, Germany. — [2]Department of Physics, Jamia Millia Islamia(Central University), New Delhi 110025, India.

In line with a recent experimental work on antiferromagnetic finite nanowires[1] and its subsequent theoretical discussions[2,3], we present here exact diagonalization calculations on the one-dimensional antiferromagnetic Heisenberg spin-$\frac{1}{2}$ chain on a magnetic substrate. The chain-substrate coupling Γ is assumed to be ferromagnetic. Numerical diagonalization is performed for chains of up to 25 spins to find the ground state and the first five excited states. The critical value of Γ at

which the ground state first changes its spin symmetry is found to be consistently higher for the odd chains as compared to the even chains considered. In odd chains, the ground state and the first excited state have the same total spin equal to $\frac{1}{2}$ whereas for even chains the ground state and the first excited state have spins 0 and 1 respectively. These bring in the premise of an odd-even effect on the ground state and low lying excited states of finite antiferromagnetic nanowires.

[1] C. F. Hirjibehedin, C. P. Lutz, A. J. Heinrich, Science **312**, 1021(2006).
[2] S. Lounis, P. H. Dederichs, and S. Blugel, Phys. Rev. Lett. **101**, 107204(2008).
[3] P. Politi and M. G. Pini, arXiv:0811.1687v1 [cond-mat.mtrl-sci].

MA 36.8 Thu 17:00 HSZ 401

Mapping of ultrafast magnetic-switch scenarios to infrared spectroscopy — •Georgios Lefkidis, Chun Li, and Wolfgang Hübner — Department of Physics and Research Center OPTIMAS, Kaiserslautern University of Technology, Box 3049, 67653 Kaiserslautern, Germany

We present a first-principles controlled ultrafast magnetooptical switch and transfer mechanism in small two-magnetic-center clusters exploiting spin-orbit-coupling enabled Λ-processes [1-4]. By attaching CO to one of the magnetic centers of the $[CoMg_2Ni]^+$ and $[CoNi]^+$ clusters and optimizing the structure we detect a mapping of the laser-induced spin manipulation to the IR spectrum of CO. The predicted spin-state-dependent CO frequencies can facilitate experimental monitoring of the processes. The lower electronic states of the clusters exhibit a very high degree of spin localization either at the Co or the Ni site. Spin flip on one magnetic atom and transfer from one magnetic center to the other are realized in structurally optimized magnetic clusters with fidelities that reach 99.8%.

[1] C. Li, G. Lefkidis and W. Hübner, arXiv:0811.4042v1 [cond-mat.other]
[2] R. Gomez-Abal, O. Ney, K. Satitkovitchai and W. Hübner, PRL 92, 227402 (2004)
[3] G. Lefkidis and W. Hübner, PRB 76, 014418 (2007)
[4] T. Hartenstein, C. Li, G. Lefkidis and W. Hübner, JPD 41, 164006 (2008).

MA 36.9 Thu 17:15 HSZ 401

Electronic theory of ultrafast spin dynamics: Towards magnetic nanologic elements — •Wolfgang Hübner[1], Sander Kersten[1,2], and Georgios Lefkidis[1] — [1]Dept. of Physics and Research Center OPTIMAS, University of Kaiserslautern, Box 3049, 67653 Kaiserslautern, Germany — [2]Dept. of Applied Physics, Eindhoven University of Technology, Box 513, 5600 MB, Eindhoven, The Netherlands

We present a fully *ab initio* theory of ultrafast nanologic elements and show that controlled spin manipulation is feasible with the inclusion of spin-orbit coupling thus realizing a Λ-process [1-3]. We discuss the requirements of such elements and we devise realistic 3-magnetic-center clusters. Out of a multitude of clusters we show, using high-level quantum chemistry, that in Ni_2Na_3 both spin flips and spin transfers are possible within a hundred femtoseconds. An external **B**-field and the state of one magnetic center serve as input bits, while the magnetic state of the cluster after a controlled laser pulse can be mapped to the result of a logic operation induced by the laser pulse. We are able to construct an OR, an XOR (CNOT) and two AND gates [4]. Thus multicenter magnetic clusters form suitable objects for extending spin dynamics to optically triggered and properly functionalized magnetic transport on a subpicosecond timescale and nanometer spatial scale.

[1] R. Gómez-Abal *et al.*, PRL 92, 227402 (2004)
[2] G. Lefkidis and W. Hübner, PRB 76, 014418 (2007)
[3] T. Hartenstein *et al.*, JPD 41, 164006 (2008)
[4] W. Hübner, S. Kersten and G. Lefkidis (unpublished)

MA 36.10 Thu 17:30 HSZ 401

Highly sensitive detection of magnetic markers by tunneling magnetoresistance sensors — •Camelia Albon, Karsten Rott, and Andreas Hütten — Thin Films and Physics of Nanostructures, Department of Physics, Bielefeld University, P.O. Box 100131, 33501 Bielefeld, Germany

Tunneling magneto-resistance (TMR) sensors are employed in the detection of magnetic markers for biological applications. An array of sensors is constructed by e-beam lithography means and consists of 20 elements placed on an 18.2 micrometer squares area. Each element has the size of 100nm on the transversal axis and 400nm on the longitudinal axis, the distance between two adjacent sensors being 1.2 micrometers. The sensors have been proved to be eligible for the detection of 1 micrometer magnetic beads by providing different detection signals with respect to the bead orientation at the sensor surface. Also, TMR sensors are able to detect the threshold of magnetic coupling between the 14nm Co nanoparticles situated on top of the sensor surface. By integrating the sensors with microchannels technique it has been proved their suitability for real time detection of magnetic markers.

MA 36.11 Thu 17:45 HSZ 401

Magnetism in homonuclear transition metal dimers — •Daniel Fritsch, Klaus Koepernik, Manuel Richter, and Helmut Eschrig — IFW Dresden, PO Box 270116, D-01171 Dresden, Germany

The present work gives an overview over calculated structural and magnetic properties of homonuclear transition metal dimers. All the calculations have been performed utilizing the full-potential local-orbital program package FPLO [1] for the solution of the Kohn-Sham equations. The ground state spin multiplicity, bond length, and harmonic vibrational frequency are obtained by scalar-relativistic calculations within the local spin-density (LSDA) and generalized gradient (GGA) approximations to the density functional. Applying the fixed-spin moment method stabilizes the convergence and helps to identify the lowest spin state. In the next step, orbital magnetic properties are obtained from spin polarized full-relativistic calculations. Since orbital moments are usually underestimated in such calculations, we have additionally studied the influence of orbital polarization corrections (OPC) [2]. The results will be compared with available experimental and other theoretical data [3].

[1] K. Koepernik and H. Eschrig, Phys. Rev. B **59**, 1743 (1999); http://www.fplo.de (version 8.00-31-WS).
[2] O. Eriksson, M. S. S. Brooks, and B. Johansson, Phys. Rev. B **41**, 7311 (1990).
[3] D. Fritsch, K. Koepernik, M. Richter, and H. Eschrig, J. Comp. Chem. **29**, 2210 (2008).

MA 36.12 Thu 18:00 HSZ 401

Stability of the magnetic domain structure of nanoparticle thin films against external fields — •Kai-Felix Braun[1], S. Sievers[1], M. Albrecht[1], U. Siegner[1], K. Landfester[2], and V. Holzapfel[2] — [1]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig. — [2]Max Planck Institute for Polymer Research, 55128 Mainz.

We investigate the influence of an external magnetic field on the magnetic ordering of single-layer and multi-layer thin films of magnetic nanoparticles (MNP). It is shown that the dipolar interaction results in a larger stability of multi-layer films as compared to single-layer films when exposed to inhomogeneous fields generated, e.g. by the magnetized tip of a magnetic force microscope (MFM). Numerical calculations and experimental MFM studies are presented. The calculations show that unperturbed single-layer MNP films display an in-plane domain pattern which is induced by dipolar interaction. Yet, even in the presence of this collective effect, external fields can rotate the spins of the MNPs out of plane. In MFM images an out-of-plane configuration manifests itself by a contrast enhancement at the film edge. This theoretical prediction is confirmed by the experimental MFM images of a single-layer film. Multi-layer films are found to be more robust against external fields than monolayers. Both calculated and measured MFM images show that the domain pattern of multi-layer films is still oberved under external fields that prevent the observation of the domain pattern of single-layer films. The nature of the collective reaction on the external perturbation will be discussed in detail and will be compared to non-interacting MNPs.