

MA 22: Magnetic Particles / Clusters II

Time: Wednesday 14:00–16:30

Location: H 1028

MA 22.1 Wed 14:00 H 1028

Magnetism in homonuclear 3d transition metal dimers — •DANIEL FRITSCH, KLAUS KOEPERNIK, MANUEL RICHTER, and HELMUT ESCHRIG — Leibniz Institute for Solid State and Materials Research IFW Dresden, PO Box 270116, D-01171 Dresden, Germany

We have investigated the structural and electronic properties of the 3d transition-metal dimers utilising the full-potential local-orbital program package FPLO [1] for the solution of the Kohn-Sham equations using the local spin density approximation (LSDA). Special emphasis has been laid on the magnetic properties of the transition-metal dimers which are obtained from spin polarised relativistic calculations. Since orbital moments are usually underestimated in these calculations we have additionally studied the influence of orbital polarisation corrections (OPC) on the orbital moments. Such corrections have been suggested by Eriksson *et al.* [2] and later in slightly modified form by Eschrig *et al.* [3]. The results will be compared with available experimental data and other theoretical investigations available in the literature.

[1] K. Koepernik and H. Eschrig, *Phys. Rev. B* **59**, 1743 (1999); <http://www.fplo.de>.

[2] O. Eriksson, M. S. S. Brooks, and B. Johansson, *Phys. Rev. B* **41**, 7311 (1990).

[3] H. Eschrig, M. Sargolzaei, K. Koepernik, and M. Richter, *Europhys. Lett.* **72** 611 (2005).

MA 22.2 Wed 14:15 H 1028

Chemical ordering and magnetic properties in bimetallic transition metal clusters — •SANJUBALA SAHOO, GEORG ROLLMANN, ALFRED HUCHT, and PETER ENTEL — Physics Department, University of Duisburg-Essen, Duisburg Campus, 47048 Duisburg, Germany

Ground state properties of binary Co-Mn icosahedral clusters are studied using the density functional theory. The structural and magnetic properties are studied with respect to various compositions of the constituents. Recent experimental observation of increase in the average magnetic moment of Co-Mn clusters with increase in Mn concentration is clearly reproduced in present studies and is related to the fact that for the smaller Co-Mn clusters with a total number of atoms, $N \leq 147$, the Mn atoms are preferably embedded on the surface of clusters. In addition, results on Co-Fe, Co-Ni and Fe-Mn clusters will also be presented.

MA 22.3 Wed 14:30 H 1028

Tuning the magnetic properties of deposited transition metal clusters by decoration — •JAN MINAR¹, S. BORNEMANN¹, H. EBERT¹, J.B. STAUNTON², S. RUSPONI³, and H. BRUNNE³ — ¹Dep. Chemie, LMU, Butenandtstr. 5-13, 81377 München, Germany — ²Department of Physics, University of Warwick, UK — ³EPF Lausanne, Switzerland

Using the fully relativistic version of the KKR-method for electronic structure calculations within local spin density functional theory (LSDA) the magnetic properties of Fe, Co and Ni clusters deposited on the Pt(111) surface have been investigated. Of central interest are the role of spin-orbit coupling as it influences the spontaneous formation and orientation of magnetic moments and gives rise amongst others to the occurrence of orbital magnetic moments, the magnetic anisotropy energy (MAE) and magnetic circular dichroism in X-ray absorption (XMCD). Our systematic investigations of different clusters and nanostructures aim to reveal the mutual relationship among their spin-orbit induced properties. In addition they show how their various magnetic properties depend on the structural properties and chemical composition of the studied system. For large two-dimensional clusters we focussed especially on the dependency of the MAE on decoration with another transition metal. Our results are in qualitative agreement with recent experimental findings. We resolved the MAE contributions for inequivalent cluster atoms and will discuss the effect of the induced MAE within the Pt substrate.

MA 22.4 Wed 14:45 H 1028

Synthesis and Characterization of Magnetic Nanoparticles — •SABRINA DISCH, WIEBKE SAGER, RAPHAËL HERMANN, GÜNTER GOERIGK, and THOMAS BRÜCKEL — Institut für Festkörperforschung,

Forschungszentrum Jülich GmbH; 52425 Jülich

Magnetic nanoparticles are the object of intensive research both because of their possible applications *e.g.* in information storage, catalysis, medical imaging and owing to the interest in fundamental understanding of their magnetic properties. Magnetic nanoparticles, as compared to bulk materials, show unique physical properties such as superparamagnetism or enhanced anisotropy constants. Very little is known about the magnetization distribution within a single particle and magnetic correlations in ordered arrangements of such nanoparticles. In order to investigate such phenomena using scattering techniques, samples of highly monodisperse nanoparticles are required.

We developed a synthesis route for the preparation of cobalt nanoparticles with diameters below 10 nm, originally based on the reduction of $Co(AOT)_2$ in water-in-oil microemulsions [1]. Our water-free synthesis route yields nanoparticle dispersions that are stable against oxidation for weeks if stored in nitrogen atmosphere. Here, we report on the progress made in synthesis optimization as well as magnetic characterization of the as-synthesized particles. We will also present results from scattering experiments performed on cobalt nanoparticles and on highly monodisperse iron oxide nanoparticles [2].

[1] C. Petit, A. Taleb, M. Pileni; *J. Phys. Chem. B*, **1999**, *103*, 1805.

[2] J. Park, T. Hyeon; *Nat. Mat.*, **2004**, *3*, 891.

MA 22.5 Wed 15:00 H 1028

Synthese von Au-core/Co-shell Nanopartikeln — •BRITTA VOGEL¹, CARSTEN WALTENBERG², INGA ENNEN¹, HARALD RÖSNER³, PETER JUTZI² und ANDREAS HÜTTEN¹ — ¹Department of Physics, University of Bielefeld, D-33615 Bielefeld, Germany — ²Department of Chemistry, University of Bielefeld, D-33615 Bielefeld, Germany — ³Institute of Nanotechnology, Forschungszentrum Karlsruhe GmbH, D-76021 Karlsruhe, Germany

Eine interessante Anwendungsmöglichkeit von magnetischen Nanopartikeln besteht im Einsatz in lebenden Zellen. Dazu ist es notwendig, die Nanopartikel mit einer biokompatiblen und oxidationshemmenden Hülle zu versehen. Eine Möglichkeit dafür bietet die Umhüllung mit Gold. [1][2]

Es wurden Cobalt-Nanopartikel durch thermische Zersetzung von Co-Precursoren synthetisiert, auf denen Gold durch Zersetzung eines Au-Precursors abgeschieden wurde. Untersuchungen der Partikel mittels HRTEM, EDX und EFTEM ergaben, dass bei dieser Synthese zunächst legierte Co/Au-Partikel als Zwischenprodukt entstehen. Es konnte experimentell durch Auslagerungsuntersuchungen gezeigt werden, dass das metastabile Zwischenprodukt in ein Au-core/Co-shell Partikel im Gleichgewichtszustand übergeht. Zudem werden magnetische Eigenschaften dieser Partikel diskutiert.

[1] R. Shenhar, V.M. Rotello, *Acc. Chem. Res.* 2003, *36*, 549. [2] M. Ch. Daniel, D. Astruc, *Chem. Rev.* 2004, *104*, 293.

MA 22.6 Wed 15:15 H 1028

Influence of biaxial stress on the magnetic properties of cobalt nanoparticles — •SRINIVASA SARANU¹, ULF WIEDWALD², PAUL ZIEMANN², and ULRICH HERR¹ — ¹Institut für Mikro- und Nanomaterialien, Universität Ulm, 89081 Ulm — ²Institut für Festkörperphysik, Universität Ulm, 89069 Ulm

Co nanoparticles with an average diameter of 25nm have been produced using an inert gas condensation technique. The particles were deposited on Si substrates and covered in situ with a 20nm Cu film. When the substrate coverage exceeds 5 %, the remanent magnetization along the in-plane direction was larger than that along the out-of-plane direction which is attributed to the dipolar interaction between the particles. For Co particles on Ta substrates, the effect of stress on the magnetic properties of isolated particles was studied. A thin film of phospholipids (DOPC) on the Ta substrate was used to avoid the agglomeration of the particles during deposition. The lipid layer was removed in an oxygen plasma, afterwards the particles were reduced to metallic Co again using a hydrogen plasma and subsequently covered with 20nm of SiO_x. The effect of stress on the magnetic properties of these particles was studied by loading the Ta substrate with hydrogen. For 0.6% of strain in the Ta substrate, out-of-plane magnetization measurements showed an increase of the saturation field H_s and a reduction of the remanent magnetization. This indicates that 25nm cobalt nanoparticles have a positive magnetostriction. Support