MA 2: Magnetic Clusters

Time: Monday 9:30–11:00 Location: HSZ 401

MA 2.1 Mon 9:30 HSZ 401

Coordination-driven magnetic-to-nonmagnetic transition in manganese doped silicon clusters — Vicente Zamudio-Bayer[1], •Linn Leppert[2], Konstantin Hirsch[1,3], Andreas Langenberg[1,3], Jochen Rittmann[1,3], Markus Kossick[1,3], Marlene Vogel[1,3], Robert Richter[3], Akira Terasaki[4], Thomas Möller[3], Bernd von Issendorff[5], Stephan Kümmel[2], and Tobias Lau[1] — [1]Institut für Methoden und Instrumentierung der Forschung mit Synchrotronstrahlung, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Theoretical Physics IV, University of Bayreuth, Germany — [3]Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany — [4]Cluster Research Laboratory, Toyota Technological Institute, Futamata, Ichikawa, Chiba, Japan — [5]Fakultät für Physik, Universität Freiburg, Germany

Using x-ray magnetic circular dichroism spectroscopy and non-empirical density functional theory we analyze the electronic, magnetic, and structural properties of manganese-doped silicon clusters. We find a correlation of the magnetic moment with the manganese coordination number and nearest-neighbor distance that indicates that high-spin states in manganese-doped silicon could be stabilized by an appropriate lattice expansion. We further discuss the necessity to correct for self-interaction errors in the underlying density functional approximation in order to predict the magnetic-to-nonmagnetic transition in accordance with experiment.

MA 2.2 Mon 9:45 HSZ 401

Laser control of ultrafast spin dynamics on homonuclear two- and three-magnetic-center clusters — •Wei Jin[1], Chun Li[2], Georgios Lefkidis[1], and Wolfgang Hübner[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Box 3049, 67653 Kaiserslautern, Germany — [2]School of Mechanics, Civil Engineering and Architecture, Northwestern Polytechnical University, Xi'an 710072, China

We present a fully *ab initio* theory for coherent laser-induced ultrafast spin manipulation on homonuclear two- and three-magnetic-center clusters.

For the homodinuclear magnetic clusters (FeOFe, FeOOFe, NiONi and NiOONi) with strong spin localizations induced by the bridging atoms, various spin flip and transfer scenarios are achieved. Out of the four clusters, the Fe-containing ones are more promising for logic operations, and this is consistent with the findings in Ref.[1].

In the pursuit of additional functionality motivated by Ref. [2] about the Co dimer, for the extended cluster Co_3^+CO we achieve a counter-clockwise cycle of spin transfer driven by three sequential laser pulses. The whole process completes within 1.2 ps, which is much faster than any conventional device. Based on this striking functionality a cyclic SHIFT register is proposed as a future application. In the strive for better magnetization dynamics control, the results on these prototypic systems strongly indicate their great potential in spintronic devices.

[1] C. Li *et al.*, Phys. Rev. B **84**, 054415 (2011).
[2] C. Li *et al.*, J. Magn. Magn. Mater. **324**, 4024 (2012)

MA 2.3 Mon 10:00 HSZ 401

The Anderson Impurity Model in Finite Systems: A Study of $CrAu_n^+$ Clusters — •Konstantin Hirsch[1], Vicente Zamudio-Bayer[1], Andreas Langenberg[1], Markus Niemeyer[1], Bruno Langbehn[2], Thomas Möller[2], Akira Terasaki[3], Bernd von Issendorff[4], and Julian Tobias Lau[1] — [1]Institut für Methoden und Instrumentierung der Forschung mit Synchrotronstrahlung, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Straße 15, 12489 Berlin, Germany — [2]Institut für Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [3]Cluster Research Laboratory, Toyota Technological Institute, 717-86 Futamata, Ichikawa, Chiba 272-0001, Japan — [4]Fakultät für Physik, Universität Freiburg, Stefan-Meier-Straße 21, 79104 Freiburg, Germany

The Anderson impurity model (AIM) describes the interaction of a magnetic impurity with the continuous density of states of a nonmagnetic host. It gives a criterium for the magnetic to nonmagnetic transition depending on two parameters: the onsite Coulomb repulsion U_0 and the hybridization strength Γ. Here we discuss the validity of the AIM in a finite host material featuring a highly discretized density of states by applying XMCD spectroscopy to size-selected $CrAu_n^+$ clusters and studying the AIM within a tight binding approach.

MA 2.4 Mon 10:15 HSZ 401

***Ab initio* thermodynamics and heat nanoengines on the magnetic Ni_2 dimer** — •Wolfgang Hübner, Chuanding Dong, Debapriya Chaudhuri, and Georgios Lefkidis — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Germany

We use the highly correlated excited electronic states of Ni_2, calculated with the symmetry-adapted-cluster configuration-interaction method, to develop thermodynamic processes and build heat engines with molecular magnets. Identifying the work of a thermodynamic process with the energy shift of the electronic- and spin levels, and the heat exchange with their population change [1] we derive an isobaric process [2] and build a Diesel and an Otto nanoengine, as well as a novel engine for which a laser pulse substitutes for the hot bath.

The many internal degrees of freedom and the nonthermal effects allow crossings of adiabatic processes in a $P-V$ diagram. We analyze the efficiency of the nanoengines and find a signifficant possible enhancement connected to the quantum nature, the spin and the heat capacity of Ni_2, as well as to the zero-field splitting of the triplet states. These new concepts connect spin dynamics with quantum thermodynamics and suggest new ways of designing effective magnetic heat-engines.
(In collaboration with J. Berakdar and L. Chotorlishvili, Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany.)

[1] M. O. Scully, Phys. Rev. Lett. **88**, 050602 (2002)
[2] C. D. Dong, G. Lefkidis and W. Hübner, J. Supercond. Nov. Magn. **26**, 1589 (2013)

MA 2.5 Mon 10:30 HSZ 401

Magnetism of sp-impurity-decorated grain boundaries and surfaces — Monika Vsianska[1,2,3], Hana Vemolova[3], and •Mojmir Sob[1,2,3] — [1]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [2]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [3]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

We present a systematic ab initio study of segregation of 12 non-magnetic sp-impurities (Al, Si, P, S, Ga, Ge, As, Se, In, Sn, Sb and Te) at $\Sigma5(210)$ grain boundary (GB) and (210) free surface (FS) in fcc ferromagnetic cobalt and nickel and analyze their effect on structure, magnetic and mechanical properties. We determine preferred segregation sites at the $\Sigma5(210)$ GB for the sp-impurities studied, their segregation enthalpies and strengthening/embrittling energies. In nickel, most of the above impurities nearly kill or substantially reduce the magnetic moments at the FS and, when segregating interstitially (i.e. Si, P, S, Ge, As, Se), also at the GB so that they provide atomically thin magnetically dead layers which may be very desirable in spintronics. Reduction of magnetic moments at the $\Sigma5(210)$ GB in fcc ferromagnetic cobalt is, in absolute values, very similar to that in nickel. However, as the magnetic moment in bulk cobalt is higher, we do not observe magnetically dead layers here. It turns out that by focused impurity segregation we can generate atomically thin magnetic layers with tailored magnetization, which can contribute to a new development of technologically important materials.

MA 2.6 Mon 10:45 HSZ 401

Tuning the magnetic anisotropy of a single nanostructure by perimetric decoration — •Marco Corbetta[1], Soo-hyon Phark[1], Jeison Antonio Fischer[1,2], Safia Ouazi[1], Dirk Sander[1], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany — [2]Laboratório de Filmes Finos e Superfícies, Departamento de Física, Universidade Federal de Santa Catarina, Florianópolis, SC, Brazil

We investigate individual Fe-decorated bilayer high Co islands on Cu(111) by spin-polarized STM in magnetic fields. Fe decorates the Co core by a few nm wide bilayer rim. This decoration induces larger switching fields Hsw of the Co cores as compared to those of pure Co islands of the same size [1,2]. The quantitative analysis of the island size dependence of the switching field reveals that all Co atoms of the Co core contribute to the magnetic anisotropy with an average value

of 0.115 meV/atom. This is 22% less than we previously reported for pure Co islands [2]. On the basis of spatially resolved measurements of the differential conductance, we ascribe this change of magnetic anisotropy to the modification of the electronic and atomic structure of the Co core due to Fe-decoration. Our spectroscopy data indicate that structural relaxations of the Co core of Fe-decorated Co islands are negligible as compared to pure Co islands, and this might be an important aspect to understand the reduced magnetic anisotropy. The Fe rim does not show a net magnetic moment, as checked by SP-STM in magnetic fields. [1] H. Oka et al., Science 327, 843 (2010). [2] S. Ouazi et al. Phys. Rev. Lett. 108, 107206 (2012).