MA 57: Focus Session "X-ray absorption spectra - state of the art of theory and experiment" (jointly with DS, HL, MM, O), Organization: Andreas Ney (Universität Duisburg-Essen)

Time: Thursday 15:15–19:00 Location: HSZ 403

Invited Talk MA 57.1 Thu 15:15 HSZ 403

Simulations of X-ray Spectra using FEFF9 and OCEAN — •John Rehr — University of Washington, Seattle, WA, USA

There has been dramatic recent progress in the theory of x-ray spectra. This spectra probes excited state properties of a system, and thus requires theoretical treatments beyond the independent particle approximation. Here we discuss two complementary approaches based on the GW/BSE method. First is a real-space Green*s function approach, as implemented in the FEFF9 code [1]. FEFF9 has improved treatments of many-body effects and can also include LDA+U corrections. Second, is a new k-space approach implemented in the GW/BSE code OCEAN (Obtaining Core Excitation using ABINIT and NBSE)[2]. OCEAN also includes intra-atomic coulomb interactions and can also treat multiplet effects. FEFF9 and OCEAN have complementary spectral ranges. However, the combination is applicable from the UV-VIS to x-ray energies. These two approaches are illustrated with applications to several core-level specra including XAS and RIXS. This work is supported by US DOE Grant DE-FG03-97ER45623 and the CMCSN. [1]J. J. Rehr et al.,Comptes Rendus Physique 10,548 (2009). [2]J. Vinson et al., arXiv:1010.0025

Topical Talk MA 57.2 Thu 15:45 HSZ 403

Polarisation dependent X-ray spectroscopy — •Andrei Rogalev, Fabrice Wilhelm, and Jose Goulon — European Synchrotron Radiation Facility (E.S.R.F.), 6 rue Jules Horowitz, 38000 Grenoble, France

In these recent years X-ray spectroscopies have been undergoing a continuous expansion, as illustrated by the discovery of a variety of new experimental techniques associated with the exploitation of the polarisation properties of synchrotron radiation. The detection of X-ray magnetic linear and circular dichroism in ferro-, ferri- and paramagnetic systems, the discovery of X-ray natural circular dichroism in gyrotropic single crystals as well as the observation of non-reciprocal X-ray linear dichroism and X-ray magneto-chiral dichroism in magnetoelectric systems are particularly interesting. In combination with sum rules these element and orbital selective spectroscopies have proved to be remarkable tools to study fundamental properties of magnetic matter via various order parameters, e.g., spin and orbital moments, electric dipole moment, orbital anapole etc. In this talk we report on advanced instrumentation developed at the ESRF beam line ID12 which is dedicated to polarization dependent x-ray spectroscopy at photon energies above 2keV. Several examples have been selected to illustrate the present performances of the beam line and to show the recent advances in the field.

Topical Talk MA 57.3 Thu 16:15 HSZ 403

Theoretical description of X-ray absorption in correlated transition metal systems — •Hubert Ebert[1], Jan Minar[1], and Ondrej Sipr[2] — [1]Ludwig-Maximilians-Universität München, Department Chemie und Biochemie, Physikalische Chemie, Butenandtstraße 11, D-81377 München, Germany — [2]Institute of Physics AS CR, Prague, Czech Republic

During the last years, great progress has been made in dealing with correlation effects in solids. Among the various theoretical approaches available now, the LSDA+DMFT (local spin density approximation + dynamical mean field theory) plays a prominent role, as it accounts for dynamical correlations when dealing with the ground state. We present a description of x-ray absorption spectra based on combining the LSDA+DMFT and the multiple scattering formalism. Working with a fully relativistic formulation, this approach gives access to a corresponding treatment of x-ray magnetic circular dichroism (XMCD). By applying the XMCD sum rules, we can demonstrate that the enhancement of orbital magnetism in ferromagnetic 3d-transition metals, which results from using the LSDA+DMFT formalism instead of plain LSDA, is indeed reflected by the XMCD spectra. Comparing the LSDA+DMFT-based XAS and XMCD spectra with experiment, however, some discrepancies remain that are ascribed to dynamical effects connected with the absorption process itself. To account for these effects we extended the sketched approach by including the presence of a core hole within the XAS and XMCD calculations using various schemes.

15 min. break

Topical Talk MA 57.4 Thu 17:00 HSZ 403

Paramagnetic molecules on metal surfaces: prototypes for spin-hybrid systems — •Heiko Wende — Faculty of Physics and CeNIDE, University of Duisburg-Essen, 47048 Duisburg, Germany

The fundamental understanding of the interaction of paramagnetic molecules with metal surfaces is crucial for the possible application of these spin-hybrid systems in molecular spintronics. We study the magnetic properties of Fe-porphyrin and Fe-phthalocyanine molecules with sub-monolayer coverages on Ni and Co films on Cu(100) with and without an intermediate layer of atomic oxygen. Dichroism in X-ray absorption spectra (XNLD and XMCD) at the respective absorption edges (Fe, Co and Ni $L_{2,3}$-edges, N and C K-edges) is investigated to identify the coupling of the molecules to the ferromagnetic layers, the orientation on the surfaces and the electronic structure. To determine the magnetic anisotropy of Fe- and Co-porphyrin molecules, the molecules were adsorbed on a non-magnetic substrate (Cu(100)). Therefore, angular-dependent XAS and XMCD spectra were measured at 5T and 8K. Calculated XAS spectra obtained from DFT and multiplet calculations using ligand field theory enable a solid interpretation of the experimental data. This work is done in collaboration with C. Weis, D. Klar, D. Bovenschen, M. Kaya, H.C. Herper, B. Krumme, A. Warland, C. Antoniak (Univ. Duisburg-Essen), M. Bernien, J. Miguel, M. Piantek, K. Baberschke, W. Kuch (FU Berlin), P. Srivastava (IIT Delhi), and B. Brena, Md. E. Ali, P.M. Panchmatia, P.M. Oppeneer, B. Sanyal, O. Eriksson (Uppsala Univ.). Supported by BMBF (05 ES3XBA/5), DFG (SFB 491 and SFB 658), STINT and ESRF(HE2700).

Invited Talk MA 57.5 Thu 17:30 HSZ 403

Can Carbon Be Ferromagnetic? — •Hendrik Ohldag[1], Elke Arenholz[2], Pablo Esquinazi[3], Daniel Spemann[3], Annette Setzer[3], Martin Rothermel[3], and Tilman Butz[3] — [1]SLAC National Accelerator Center — [2]Lawrence Berkeley National Laboratory — [3]University Leipzig

The existence of long range magnetic order at room temperature in carbon based structures without magnetic elements is very unexpected. Theoretical results from different groups suggest that the existence of long range magnetic order in a graphite structure is possible, if one takes the effects of defects and/or the incorporation of hydrogen atoms into account. SQUID results provided first systematic hints for the existence of magnetic order at room temperature in virgin as well as irradiated graphite samples. We present a x-ray dichroism study of graphite surfaces [1] that addresses the origin and magnitude of ferromagnetism in metal-free carbon. Using element specific x-ray microscopy we can show that metallic impurities do not play a role in the ferromagnetism of carbon and that carbon can be ferromagnetic without ferromagnetic impurities. A detailed spectroscopic study shows that in addition to carbon pi-states, also hydrogen-mediated electronic states exhibit a net magnetization with magnetic remanence at room temperature. The observed magnetism is restricted to the top ~10 nm of the sample where the actual magnetization reaches a value similar to that of Nickel. [1] H. Ohldag et al., Phys. Rev. Lett. 98, 187204 (2007) and to appear in New. Jour. Phys. (2011).

MA 57.6 Thu 18:00 HSZ 403

Investigation of strain and doping induced ferromagnetism in $LaCoO_3$ by x-ray absorption and magnetic circular dichroism — Michael Merz[1], Peter Nagel[1], Andrea Assmann[1,2], Stephan Uebe[1,2], Markus Wissinger[1,2], Hilbert von Löhneysen[1,3], Dirk Fuchs[1], and •Stefan Schuppler[1] — [1]Institut für Festkörperphysik, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]Fakultät für Physik, Karlsruhe Institute of Technology — [3]Physikalisches Institut, Karlsruhe Institute of Technology, 76031 Karlsruhe, Germany

Undoped bulk $LaCoO_3$ remains paramagnetic down to liquid He temperatures; it has been shown that upon cooling, the Co^{3+} ions undergo a spin-state transition to the $S = 0$ low-spin (LS) state. We explore two avenues for inducing ferromagnetism in this compound: (i) strain, applied by the lattice mismatch between a $LaCoO_3$ thin film and the

substrate, and (ii) doping, both with electrons and holes. The spin-state structure of these systems can be studied in detail by near-edge x-ray absorption fine structure and by soft x-ray magnetic circular dichroism at the Co $L_{2,3}$ and the O K edges. It turns out that the mechanism responsible for ferromagnetism in each of the systems – strained undoped, electron doped, hole doped – is unique and distinctly different from the others, explaining the vastly differing transition temperatures. In all cases, a mix of Co spin states is realized, and thus their actual microscopic arrangement is a co-determining factor for magnetic parameters like the spin and orbital moments.

MA 57.7 Thu 18:20 HSZ 403

Ab initio study of surface and interface effects on XANES and XMCD of Fe/BaTiO3 systems — •Stephan Borek[1], Angelika Chassé[1], Remya Kunjuveettil Govind[1], Vasili Hari Babu[2], Federica Bondino[3], Martin Trautmann[1], Marco Malvestuto[3], Karl-Michael Schindler[1], Reinhard Denecke[2], Igor Maznichenko[1], and Arthur Ernst[4] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany — [2]Wilhelm-Ostwald Institute for Physical and Theoretical Chemistry, University Leipzig, Germany — [3]IOM CNR, Laboratorio Nazionale TASC, Area Science Park, Basovizza, Italy — [4]Max-Planck-Institut für Mikrostrukturphysik Halle

The aim of our work is the spectroscopic characterization of multiferroic heterostructures by means of x-ray absorption spectroscopy (XAS). Starting form first-principles calculations of bulk $BaTiO_3$ (BTO) the influence of surface and surface termination of BTO on x-ray absorption near edge structure (XANES) and x-ray magnetic circular dichroism (XMCD) is studied for different edges in BTO. In the case of iron layers on BTO, effects at the interface and of layer thickness on XANES and XMCD are considered by means of layer-resolved contributions within a multi-code approach. Calculations are shown in dependence on the direction of polarization of ferroelectric BTO (tetragonal phase). The calculated results are compared to experimental data.

MA 57.8 Thu 18:40 HSZ 403

Co-doped ZnO epitaxial films: signs of phase separation by means of hard x-ray absorption spectroscopy — •Verena Ney, Shunagli Ye, Katharina Ollefs, Tom Kammermeier, and Andreas Ney — Fakultät für Physik and CeNIDE, Universität Duisburg-Essen, 47057 Duisburg, Germany

X-ray absorption spectroscopy (XAS) using linear and circular polarized light offers a powerful toolbox of element-specific structural, electronic, and magnetic probes that is especially well suited for studying $Zn_{1-x}Co_xO$ (Co:ZnO) to unravel its intrinsic properties. We demonstrate that as long as phase separation or excessive defect formation is absent, Co:ZnO is paramagnetic [1]. We can establish quantitative thresholds based on four reliable quality indicators using XAS; samples which show ferromagnet-like behaviour fail to meet these quality indicators, and complementary experimental techniques indeed prove phase separation [2]. Careful analysis of XAS spectra is shown to provide valuable information of secondary phases in a highly sensitive, non-destructive manner.

[1] A. Ney et al., Phys. Rev. Lett. **100**, 157201 (2008).

[2] A. Ney et al., New J. Phys. **12**, 013020 (2010).

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