A 37: Atomic clusters

Time: Thursday 14:00–16:00 Location: V57.05

Invited Talk A 37.1 Thu 14:00 V57.05

X-ray magnetic circular dichroism spectroscopy of size-selected free cluster ions: spin coupling, orbital angular momentum quenching, and magnetic dopants — •Tobias Lau — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Methoden und Instrumentierung der Forschung mit Synchrotronstrahlung, Albert-Einstein-Straße 15, 12489 Berlin

X-ray magnetic circular dichroism (XMCD) spectroscopy is a local and element specific probe to study spin and orbit contributions to the total magnetic moment. With a 5 T and 15 K linear ion trap setup we have sucessfully applied XMCD of size selected cluster ions to study fundamental magnetic properties of transition metals in the molecular limit. Recent results include the observation of ferromagnetic spin coupling in small clusters of archetypical bulk antiferromagnets, as well as antiferromagnetic spin coupling in iron, the most typical 3d bulk ferromagnet. We could also show that the orbital angular momentum is largely quenched already for the smallest iron clusters. Furthermore, magnetization curves recorded at fixed ion trap temperature can be used to determine the cluster ion temperature. As an outlook, first results of XMCD spectroscopy of single impurity atoms in size selected clusters ions will be presented.

Invited Talk A 37.2 Thu 14:30 V57.05

Autoionization of clusters: Energy transfer vs. electron transfer — •Uwe Hergenhahn — Max-Planck-Institut für Plasmaphysik, EURATOM Association, 85748 Garching

In this talk I will give a progress report about our experimental work on autoionization of clusters. The discovery of autoionizing decays into charge separated two-hole sites in clusters (Interatomic/Intermolecular Coulombic Decay, ICD) has been followed by experiments, in which such decays are mediated by charge transfer between sites (Electron Transfer Mediated Decay, ETMD). For ICD, which proceeds by energy transfer, evidence for the occurence of this process as a second step in a cascade after normal Auger decay of water clusters will be presented. For ETMD, the interpretation of outer valence and electron,electron coincidence spectra allows to get a comprehensive picture of this autoionization channel in ArXe clusters of varying size.

A 37.3 Thu 15:00 V57.05

First-order corrections and structural information in semiclassical Gaussian approximations to the Boltzmann operator for clusters of atoms — •Holger Cartarius[1] and Eli Pollak[2] — [1]1. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Chemical Physics Department, Weizmann Institute of Science, 76100 Rehovot, Israel

Gaussian approximations to the Boltzmann operator have proven themselves in recent years as useful tools for the study of the thermodynamic properties of rare gas clusters. They are, however, not necessarily correct at very low temperatures. We introduce a numerically cheap frozen Gaussian approximation to the imaginary time propagator with a width matrix especially suited for the dynamics of clusters [1] and investigate its first-order correction to diagnose the quality of the approximation [2]. The strength of the correction to the Gaussian partition function monitored as a function of the temperature indicates that the results of the Gaussian propagator become questionable below a certain temperature, however, thermodynamic henomena such as structural transformations occur in a temperature range for which the Gaussian approximation is predicted to be accurate.

To study transformations or dissociation effects of rare gas clusters for increasing temperature information about the structure is essential. We show how structural information can be extracted from the Gaussian imaginary time propagator.

[1] H. Cartarius, E. Pollak, J. Chem. Phys. 134, 044107 (2011)
[2] H. Cartarius, E. Pollak, Chem. Phys., in press (2011)

A 37.4 Thu 15:15 V57.05

Core-level photoelectron spectroscopy on free mass-selected Gold clusters at the free-electron laser FLASH — •Patrice Oelssner[1], Jens Bahn[1], Michael Köther[1], Christian Braun[2], Volkmar Senz[1], Steffen Palutke[3], Michael Martins[3], Gerd Ganteför[2], Bernd von Issendorff[4], Josef Tiggesbäumker[1], and Karl-Heinz Meiwes-Broer[1] — [1]IfPh, Uni-Rostock — [2]FB Physik, Uni-Konstanz — [3]IfExp. Physik, Uni Hamburg — [4]Fak. f. Physik, Uni Freiburg

A promising method to investigate the electronic structure of clusters is core-level photoelectron spectroscopy as used extensively in surface science [Phys. Rev. Lett. 102, 138303 (2009)]. The VUV free electron laser FLASH at DESY delivers intense light with a wavelength down to 4.8 nm (258 eV) to allow such studies. With a hemispherical analyzer equipped with a Delay-Line-Detector we studied core-level-binding energies. Results on mass-selected gold clusters anions from 45 to 150 atoms show a size-dependent 4f core-level shift as predicted by the metal sphere model [Phys. Rev. B 50,5744 (1994)]. By measuring the gold 4f binding energies of anions and cations as a function of cluster-size one can calculate, e.g. the chemical potential.

A 37.5 Thu 15:30 V57.05

Core level photoelectron spectroscopy on free mass-selected lead clusters at FLASH — •Jens Bahn[1], Patrice Oelssner[1], Michael Köther[1], Christian Braun[3], Volkmar Senz[2], Steffen Palutke[4], Bernd von Issendorff[5], Gerd Ganteför[3], Michael Martins[4], Josef Tiggesbäumker[1], and Karl-Heinz Meiwes-Broer[1] — [1]Institut für Physik, Universität Rostock — [2]Institut für Biomedizinische Technik, Universität Rostock — [3]Fachbereich Physik, Universität Konstanz — [4]Institut für Experimentalphysik, Universität Hamburg — [5]Fakultät für Physik, Universität Freiburg

The electronic structure forms the basis for understanding the physical and chemical properties of clusters. A promising method to study this issue is core-level photoelectron spectroscopy using the VUV free electron laser FLASH at DESY providing wavelengths down to 4.8 nm. Results on lead clusters feature size-dependent 5d and 4f core-level shifts and reveal a remarkable change of final state screening conditions due to a metal to nonmetal transition at cluster sizes about 20 atoms [Phys. Rev. Lett. 102, 138303 (2009)]. In recent experiments a hemispherical electron spectrometer has been utilized. It became possible to allocate electron signals to each micro pulse of FLASH with a time-resolved delay-line-detector. A sequence of cluster sizes can be probed by this approach. By study of 4f core-level of lead clusters the change of the gaussian line shape to a Doniach-Sunjic profile has been observed as function of size. The evolution of the line profiles can be understood as scattering processes in finite systems.

A 37.6 Thu 15:45 V57.05

Spin Coupling and Orbital Momentum Quenching in Small Iron and Cobalt Clusters — •Andreas Langenberg[1,2], Konstantin Hirsch[1,2], Vicente Zamudio-Bayer[1,2], Markus Niemeyer[1,2], Arkadiusz Lawicki[2], Marlene Vogel[2], Kazuhiro Egashira[3], Thomas Möller[2], Akira Terasaki[3], Bernd von Issendorff[4], and Tobias Lau[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert Einstein Str. 15, 12489 Berlin — [2]Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin — [3]Cluster Research Laboratory, Toyota Technological Institute, Ichikawa 272-0001, Japan — [4]Universität Freiburg, Fakultät für Physik, 79104 Freiburg, Germany

X-ray magnetic circular dichroism (XMCD) spectroscopy was performed on free and size selected iron and cobalt clusters in a linear penning trap giving direct access to spin and orbital resolved magnetic moments (m_s, m_l). For iron clusters a quenching of the orbital magnetic moments for already very small clustersizes and an antiferromagnetic coupling of Fe_{13}^{+} [1] can be observed. Moreover the measured total magnetic moments of the clusters $(m_j = m_l + m_s)$ are in good agreement with results from Stern-Gerlach experiments [2,3]. High resolution XMCD spectra as well as magnetization curves of cobalt and iron clusters will be discussed in detail.

[1] P. Bobadova-Parvanova, K. A. Jackson et.al., Phys. Rev. B 66, 195402 (2002)
[2] X. Xu, S. Yin et.al., Phys. Rev. Lett. 95, 237209 (2005)
[3] M. Knickelbein, Chem. Phys. Lett. 353, 221-225 (2002)