SYPE 2 SYPE II

Zeit: Freitag 16:30–19:00 Raum: HU Senatssaal

Hauptvortrag SYPE 2.1 Fr 16:30 HU Senatssaal

From Einstein's Photoelectric Effect to ZEKE Rydberg States and a New Molecular Orbital Description — •Klaus Müller-Dethlefs — York Centre for Laser Spectroscopy, Department of Chemistry — The University of York, York YO10 5DD, United Kingdom

From Einstein's discovery of the photo-electric effect, one of the pillars of modern quantum theory, it has taken nearly fifty years until the first practical application of the photoelectric effect to molecules was demonstrated in the 1960's by David Turner at Imperial College. The main advance came from the discovery of a very high intensity He(I) light source. Another twenty years later, we developed rotationally resolved ZEKE (Zero Electron Kinetic Energy) photoelectron spectroscopy, based on the pulsed field ionization of long-lived, very high n, Rydberg states and, over the last two decades, refined it as a valuable tool for the study of molecular ions and clusters. Here we present a new useful definition for molecular orbitals that is based on the analysis of rotationally resolved ZEKE spectra. The selection rules for ZEKE transitions from a neutral molecule of total angular momentum (J) to an ion core (J+) and a Rydberg electron (l) are more complicated than for neutral transitions since angular momentum is transferred to the final state ZEKE Rydberg electron. Hence for the rotational band contour analysis of ZEKE spectra a suitable model must be employed to account for the ionisation dynamics. In the model presented here we find that the overlap of the ion ground state wave-function with the neutral state wave-function leads to an unambiguous definition of the HOMO of the neutral state. We call this orbital a spectator orbital since it is coupled to a fully electronically relaxed ion wave-function. The orbital, which is related to the "Dyson"orbital, is well defined for any level of theory used to compute the electronic wavefunctions of the neutral or of the ion.

Hauptvortrag SYPE 2.2 Fr 17:00 HU Senatssaal

Time-dependent photoelectron spectroscopy — •Daniel Neumark — Department of Chemistry, University of California, Berkeley, CA 94720 USA

Time-resolved photoelectron imaging (TRPEI) is applied to the study of dynamics in size-selected anion clusters. Results will be presented for mercury and water cluster anions. In the mercury cluster experiments, TRPEI is used to follow relaxation dynamics subsequent to intraband excitation of the excess p-electron. In the water cluster anions, we show that internal and surface states can be selectively generated and measures size-dependent internal conversion lifetimes for the electronically excited "p"state in both types of clusters. Extrapolation of our results for the internal states supports the non-adiabatic relaxation model proposed for bulk hydrated electrons.

Hauptvortrag SYPE 2.3 Fr 17:30 HU Senatssaal

Phasen- und zeitaufgelöste Photoelektronenspektroskopie an Atomen und Festkörpern — •Ulrich Heinzmann — Fak. Physik, Universität Bielefeld, 33501 Bielefeld

Der Vortrag gibt über jüngst durchgeführte Experimente zeitaufgelöster Photoelektronenspektroskopie an freien Atomen (Zeitauflösung 250 as /1/) und zeitaufgelöster Photo-ESCA an Festkörperoberflächen (Zeitauflösung 50 fs /2,3/) einen Überblick. Auch wenn ein einzelnes Photon keine Phase besitzt, so ist die Phasenlage der elektromagnetischen Schwingungen in einem ultrakurzen as- bzw. fs-Puls experimentell einstellbar und messbar /4/. Auch wird über die experimentelle Bestimmung von Phasendifferenzen der Photoelektronenwellenfunktionen mittels spinaufgelöster Untersuchungen des Photoeffektes an Atomen /5/ und Festkörperoberflächen /6/ berichtet.

/1/ E. Goulielmakis et al. Science 305, 1267 (2004)
/2/ P. Siffalovic et al. Europhys. Lett. 60, 924 (2002)
/3/ P. Siffalovic et al. J. Biotechn. 112, 139 (2004)
/4/ R. Kienberger et al. Nature 427, 817 (2004)
/5/ G. Snell et al. Phys. Rev. A 63, 032712 (2001)
/6/ N. Müller et al. J. Electr. Spectr. 114,777 (2001)

Hauptvortrag SYPE 2.4 Fr 18:00 HU Senatssaal

The Electronic Structure of Charged Matter: Photoionization of Positive and Negative Ions — •Nora Berrah — Physics Department, Western Michigan University, Kalamazoo, Mi, USA

Prior to third generation light sources, the electronic structure of charged matter was investigated in Europe via challenging photoionization studies of positive ions [1, 2], due to tenuous targets and low photon flux. The new and improved light sources have allowed a rebirth in fundamental studies of photon-matter interactions, and in particular of the electronic structure and dynamics of negative and positive ions.

We will present at the symposium, new unprecedented results of photoionization studies in both positive and negative ions conducted at Super-ACO, France [3], ASTRID, Denmark [4], and the ALS [5, 6], USA. Specifically, the electronic dynamics was examined, including the mechanisms of electronic decay processes of multi-excited states, nuclear dynamics and structure. This work will in general extend our quantum mechanical understanding of complex systems.

References:

[1] I. C. Lyon *et al.*, J. Phys. B. **19**, 4137 (1986).
[2] F. Wuilleumier, in AIP Conf. Proc. No. **119**, New York pp 220-232.
[3] J.-M. Bizau *et al.*, Phys. Rev. Lett. **87**, 273002 (2001).
[4] H. Kjeldsen *et al.*, J. Phys. B. 34, L353 (2001); T. Andersen, Physics Report, 394, 157 (2004).
[5] A. A. Covington *et al.*, Phys. Rev. Lett. **87**, 243002 (2001); J. Phys. B. **34**, L735 (2001).
[6] N. Berrah *et al.*, PRL **87**, 253002 (2001); PRL **88**, 093001 (2002).

Hauptvortrag SYPE 2.5 Fr 18:30 HU Senatssaal

Multiphotonionisation von Atomen und Clustern mit weicher Röntgenstrahlung — •Thomas Möller — Institut für Atomare Physik und Fachdidaktik, Technische Universität Berlin

Durch optisch nicht-lineare Prozesse können Atome und Moleküle auch mit niederenergetischen Photonen ionisiert werden. Neuartige besonders leistungsfähige Lichtquellen wie Freie-Elektronen Laser (FEL) liefen kurzwellige Femtosekunden-Lichtpulse im Bereich von VUV- und weicher Röntgenstrahlung. Sie bieten vollständig neue Forschungsmöglichkeiten und erlauben es nicht-lineare Prozesse mit hochenergetischen Photonen zu induzieren [1]. Im Vortrag wird über erste Ergebnisse an Atomen und Clustern berichtet, die mit einem VUV-FEL erzielt wurden. Einfach und-Multiphotonabsorption führt in Atomen und Clustern zu hohen Ladungszuständen. Es zeigt sich, dass bei kurzen Wellenlängen die im optischen Spektralbereich dominanten Feldionisation (Tunnelionisation) keine nennenswerte Rolle spielen. Zukünftige Forschungsprojekte werden im Ausblick vorgestellt.

1 T. Laarmann, H. Wabnitz, J. Schulz, A.R.B. de Castro, P. Gürtler, W. Laasch, T. Möller, Phys. Rev. Lett. 92, 143401