

## O 88: Electronic structure II

Time: Friday 10:30–13:00

Location: MA 043

O 88.1 Fri 10:30 MA 043

**The XPS-limit in Hard X-ray Angle Resolved Photo emission** — ●JÜRGEN BRAUN, JAN MINAR, and HUBERT EBERT — Universität München, Department Chemie, Butenandtstr. 5-13, D-81377 München, Germany

A brief introduction to the theory of angle-resolved photo electron spectroscopy (ARPES) of solid materials is given with an emphasis on the so-called one-step-model of photo emission that describes excitation, transport to the surface and the escape into the vacuum in a coherent way. The main aspects of the theory and its implementation within the Munich SPR-KKR program package [1] will be reviewed. As a new feature we present a model that accounts for finite temperatures when calculating photo emission spectra on the basis of the Coherent Potential Approximation (CPA) alloy theory (alloy analogy model). Our method goes well beyond the simple, but standard Debye-Waller approach to photo emission by including in particular the temperature dependence of the effective photo emission matrix elements as well. This allows among others to reproduce the so called XPS- or density of states limit in angle-resolved photo emission which occurs for high photon energies and/or high temperatures due to a full Brillouin zone averaging caused by phonon scattering. To illustrate the applicability of the new formalism examples of soft- and hard X-ray ARPES calculations for W(110), Pt(111) and Au(111) will be presented.

1. H. Ebert et al., The Munich SPR-KKR package, version 5.4, <http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR> (2009)

O 88.2 Fri 10:45 MA 043

**Spin- and angle-resolved photoemission spectroscopy on Bi<sub>2</sub>Te<sub>3</sub> thin films** — ●ALEXEJ HERDT<sup>1</sup>, LUKASZ PLUCINSKI<sup>1</sup>, GUSTAV BIHLMAYER<sup>1</sup>, GEORG MUSSLER<sup>1,2</sup>, SVEN DÖRING<sup>3</sup>, DETLEV GRÜTZMACHER<sup>1,2</sup>, STEFAN BLÜGEL<sup>1</sup>, and CLAUS MICHAEL SCHNEIDER<sup>1,2,3</sup> — <sup>1</sup>Peter Grünberg Institut, Forschungszentrum Jülich — <sup>2</sup>Jülich Aachen Research Alliance - Fundamentals of Future Information Technologies (JARA-FIT), Forschungszentrum Jülich — <sup>3</sup>AG Prof. Dr. C.M. Schneider, University Duisburg-Essen

Recently, topological insulators have attracted wide attention in the field of condensed matter physics. Typical materials showing the topological phase are Bi<sub>1-x</sub>Sb<sub>x</sub>, Bi<sub>2</sub>Se<sub>3</sub> or Bi<sub>2</sub>Te<sub>3</sub>, which have been theoretically predicted and experimentally observed in several studies [1]. We investigate the surface state spin texture of an epitaxial MBE-grown Bi<sub>2</sub>Te<sub>3</sub>/Si(111) thin film using angle- and spin-resolved photoelectron spectroscopy (SP-ARPES). Film growth and characterization are described elsewhere [2,3]. Our study shows, that the linear Dirac cone is accompanied by deeper lying high spin-polarized energy dispersive surface states up to 4 eV binding energy. These states indicate clear reversals of the spin vector components for both chiralities measured on different Fermi surface positions located in the **k**-space. The results are supported by our high-resolved ARPES data as well as theoretical *ab initio* band structure calculations in thin film geometry.

[1] M. Z. Hasan *et al.*, Rev. Mod. Phys. 82, 3045 (2010)

[2] J. Krumrain *et al.*, J. Cryst. Growth 324, 115 (2011)

[3] L. Plucinski *et al.*, Appl. Phys. Lett. 98, 222503 (2011)

O 88.3 Fri 11:00 MA 043

**Electronic structure of spatially aligned graphene nanoribbons** — ●STEFFEN LINDEN<sup>1</sup>, DINGYONG ZHONG<sup>1</sup>, ALEXANDER TIMMER<sup>1</sup>, HAIMING ZHANG<sup>1</sup>, NABI AGHDASSI<sup>1</sup>, XINLIANG FENG<sup>2</sup>, KLAUS MÜLLEN<sup>2</sup>, HARALD FUCHS<sup>1</sup>, HELMUT ZACHARIAS<sup>1</sup>, and LIFENG CHI<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — <sup>2</sup>Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

On-surface covalent coupling under UHV conditions is a new concept to create robust, ordered molecular surface structures that may also exhibit novel properties [1]. Starting from specifically designed primer molecules, well-orientated armchair graphene nanoribbons (aGNRs) with well-defined widths have been obtained on a stepped gold surface. To study the structural and electronic properties of these GNRs, scanning tunneling spectroscopy (STM), angle-resolved ultraviolet photoemission spectroscopy (ARUPS) and inverse photoemission (IPE) have been conducted. STM shows the exclusive presence of 7-aGNRs and a few percent of 13-aGNRs on the substrate. The combination of

ARUPS and IPE reveals bandgaps of 2.8 eV and 1.6 eV for 7-aGNRs and 13-aGNRs, respectively. These values are in between those obtained from LDA and GW calculations for freestanding aGNRs[2,3]. Thus a weak doping from the underlying gold substrate may occur. These results clearly show the development of a sizable bandgap in narrow aGNRs.

[1] J. Cai *et al.*, Nature 466, 470 (2010), [2] J. W. Son *et al.*, PRL 97, 216803 (2006), [3] Li Yang *et al.*, PRL 99, 186801 (2007)

O 88.4 Fri 11:15 MA 043

**Co thin films on Cu(001): dispersion and spin polarisation of the unoccupied quantum well state** — ●MARTIN ELLGUTH, CHRISTIAN TUSCHE, AIMO WINKELMANN, and JÜRGEN KIRSCHNER — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

Co thin films on Cu(001) are a thoroughly investigated material system, where a surface state is present and quantum well states occur in the unoccupied part of the band structure. Using our momentum microscope, we have measured energy-resolved momentum images in two-photon photoemission (2ppe:  $h\nu = 3.1$  eV) using 400-nm-photons from a frequency doubled Ti:Sa laser. The momentum imaging principle yields the full  $k_{||}$ -space of photoelectrons in a single measurement. We assemble such images over a range of kinetic energies and select an energy-vs- $k_{||,1}$  cut from the 3-dimensional dataset to visualize the dispersion relation of the unoccupied quantum well states in 2ppe depending on the film thickness (3 to 11 monolayers).

For a selected initial energy of 350 meV below the Fermi level, we obtain a spin-polarised version of such an image by placing a recently developed 2-dimensional imaging spin detector<sup>1</sup> into the electron beam path. We observe a spin polarisation of 0.5 for those  $k_{||,1}$ , where the resonant excitation via the quantum well state yielded an increased intensity and 0.45 in the remaining  $k_{||}$ -regions.

[1] C. Tusche, M. Ellguth, A.A. Ünal, C.-T. Chiang, A. Winkelmann, A. Krasnyuk, M. Hahn, G. Schönhense, J. Kirschner, *Appl. Phys. Lett.* **99**, 032505 (2011)

O 88.5 Fri 11:30 MA 043

**Low-Energy Scale Excitations in the Spectral Function of Organic Monolayer Systems** — ●ACHIM SCHÖLL<sup>1,2</sup>, JOHANNES ZIROFF<sup>1,2</sup>, SIMON HAME<sup>1,2</sup>, MARIO KOCHLER<sup>1,2</sup>, AZZEDINE BENDOUNAN<sup>1,2</sup>, and FRIEDRICH REINERT<sup>1,2</sup> — <sup>1</sup>Experimentelle Physik VII und Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, 97074 Würzburg, Germany — <sup>2</sup>Gemeinschaftslabor für Nanoanalytik, Karlsruher Institute für Technologie KIT, 76021 Karlsruhe, Germany

Using high-resolution photoemission spectroscopy we demonstrate that the electronic structure of several organic monolayer systems, in particular 1,4,5,8-naphthalene tetracarboxylic dianhydride and Copperphthalocyanine on Ag(111), is characterized by a peculiar excitation feature right at the Fermi level. This feature displays a strong temperature dependence and is immediately connected to the binding energy of the molecular states, determined by the coupling between the molecule and the substrate. At low temperatures, the line-width of this feature, appearing on top of the partly occupied LUMO (lowest unoccupied molecular orbital of the free molecule), amounts to only  $\sim 10$ meV, representing an unusually small energy scale for electronic excitations in these systems. We discuss possible origins, related e.g. to many-body excitations in the organic-metal adsorbate system, in particular a generalized Kondo scenario based on the single impurity Anderson model.

O 88.6 Fri 11:45 MA 043

**In situ angle resolved photoelectron spectroscopy (ARPES) during the formation and depth sensitive hard X-ray photoelectronspectroscopy (HAXPES) of a ZnO:Ni nanocomposite** — ●ARNDT QUER, ERIK KRÖGER, MATTHIAS KALLÄNE, LUTZ KIPP, and KAI ROSSNAGEL — Institute of Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany

Magnetolectric composites based on piezoelectric and magnetostrictive substances have drawn significant interest in recent years due to their multifunctionality and potential technological aspects, e.g. sensor applications. For the magnetolectric coupling the interface between the

two components and its magnetic and electronic structure is of basic interest. The composite of magnetostrictive Ni thin films on top of piezoelectric ZnO-substrates was used as a simple basic system. In order to investigate the electronic structure during interface formation, we performed in situ photoelectron spectroscopy (PES), revealing NiO formation at the interface and in addition charge transfer from the Ni adatoms to the ZnO substrate. The resulting enhanced conductivity of the ZnO surface enables high resolution ARPES measurements. These ARPES results of the electronic structure of the composite over the Brillouin zone in  $\Gamma$ MK-plane are shown. Furthermore the "complete" composite of a 5 nm thin film nickel on ZnO substrate was investigated by depth sensitive HAXPES. This work was supported by the DFG via SFB855.

O 88.7 Fri 12:00 MA 043

**Extremely short mean free path of electrons in lanthanides** — •KAREN ZUMBRÄGEL, ANKE B. SCHMIDT, and MARKUS DONATH — Physikalisches Institut, WWU Münster

The probing depth of electron spectroscopies is determined by the mean free path of electrons within the investigated material. Schönhense and Siegmann predicted a rule of thumb that for transition metals the electron mean free path for low energies is inversely proportional to the number of d holes [1]. This rule was confirmed for, e.g., Fe with 3 to 5 monolayers [2] and predicts an extremely short mean free path of less than 1 ML for Gd.

We performed overlayer experiments with gadolinium and terbium grown on tungsten. Applying inverse photoemission, we observed the decreasing intensity of tungsten bulk-state transitions as a function of the lanthanide film thickness. Thus we were able to determine the mean free path for low-energy electrons in gadolinium and terbium and confirm therewith the prediction of Schönhense and Siegmann.

[1]Schönhense and Siegmann, *Ann. Phys.* 2 (1993) 465

[2]Passek et al., *J. Magn. Magn. Mat.* 159 (1996) 103

O 88.8 Fri 12:15 MA 043

**Charge transfer and dipole-dipole repulsion at ultra-thin organic heterojunction on metal** — •PATRICK AMSALEM<sup>1</sup>, JENS NIERDERHAUSEN<sup>1</sup>, ANDREAS WILKE<sup>1</sup>, RAPHAEL SCHLESINGER<sup>1</sup>, STEFANIE WINKLER<sup>1</sup>, ANTJE VOLLMER<sup>2</sup>, JURGEN P. RABE<sup>1</sup>, and NORBERT KOCH<sup>1</sup> — <sup>1</sup>Humboldt-Universität zu Berlin, Institut für Physik, Newtonstrasse 15, Berlin 12489, Germany — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH - BESSY II, Albert-Einstein-Strasse 15, Berlin 12489, Germany

We investigate the electronic properties of a two monolayer thick organic heterojunction grown on a metal surface by photoelectron spectroscopy. The first molecular  $\alpha$ -sexithiophene layer is physisorbed on the Ag(111) substrate and the sample work function decreases by 0.7 eV. Upon incremental deposition of an organic C60 overlayer, a charge

transfer state, attributed to the partial filling of the C60 LUMO-derived states, is observed. This is accompanied by a work function increase which does not increase linearly as a function of coverage within the sub-monolayer regime. Analysis of the valence band and core level spectra reveals that the overlayer is actually composed of a mixture of charged and neutral species. Noteworthy, the work function behavior is correlated with the ratio of charged and neutral molecules, which depends on coverage. Dipole-dipole repulsion is proposed as the main driving force to explain these charge/neutral molecule ratio variations. The energy level alignment and structural properties are discussed by invoking simple electrostatic considerations.

O 88.9 Fri 12:30 MA 043

**Localized Doping on an Atomic Chain System** — •I. BARKE, S. POLEI, V. V. OEYNHAUSEN, and K.-H. MEIWES-BROER — Institut für Physik, Universität Rostock, 18051 Rostock, Germany

Adatoms can be used as efficient dopants for band-structure engineering of surfaces. While delocalized electron waves in two or three dimensions are usually affected by an ensemble of impurities, perfect separation of segments between two dopants can be achieved in one dimension. This results in local regions of well-defined charge-carrier concentrations. On the quasi one-dimensional system Si(111)5x2-Au it is shown that quantum wires between two doping adatoms establish a local electronic structure depending on the respective adatom distance. Within a chain segment the effect of a spatially independent charge-carrier concentration is superimposed by a Coulomb-like interaction with the positively charged impurities. This offers a natural explanation for the relatively broad features observed in photoemission [1] and the complex appearance in STM and STS images [2].

[1] J. L. McChesney et al., 70, 195430 (2004).

[2] I. Barke et al., *Solid State Commun.* 142, 617 (2007).

O 88.10 Fri 12:45 MA 043

**Doped silicene: Evidence of a wide stability range** — •UDO SCHWINGENSCHLÖGL, YINGCHUN CHENG, and ZHIYONG ZHU — KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia

The effects of doping on the lattice structure, electronic structure, phonon spectrum, and electron-phonon coupling of low-buckling silicene are studied by first-principles calculations. Although the lattice is found to be very sensitive to the carrier concentration, it is stable in a wide doping range. The frequencies of the G and D Raman modes can be used to probe the carrier concentration. In addition, the phonon dispersion displays Kohn anomalies at the  $\Gamma$  and K points which are reduced by doping. This implies that the electron-phonon coupling cannot be neglected in field-effect transistor applications.

Reference: *EPL* **95**, 17005 (2011).