O 85: Electron and spin dynamics I

Time: Thursday 16:30–19:00 Location: WIL A317

O 85.1 Thu 16:30 WIL A317

Electron-phonon coupling in laser excited metals — •Isabel Klett, Benedikt Müller, and Bärbel Rethfeld — TU Kaiserslautern, Germany

Irradiation of metals with an ultrashort laser pulse leads to a hot electron gas while the lattice stays cold. The corresponding electron-phonon coupling has been calculated using a thermalized Fermi distribution function [1]. However, after laser excitation, the electrons cannot be assumed in equilibrium, due to their relaxation time of tens of femtoseconds. In order to allow a nonequilibrium distribution function, the Boltzmann equation is applied [2]. This model is extended by implementing the density of states of real metals into the Boltzmann collision terms. From the solution we extract the electron-phonon coupling in thermal nonequilibrium.

[1] Z. Lin, L. Zhigilei and V. Celli in Phys.Rev.B **77**, 075133 (2008)
[2] B. Rethfeld, A. Kaiser, M. Vicanek and G. Simon in Phys.Rev.B **65**, 214303 (2002)

O 85.2 Thu 16:45 WIL A317

Dangling-bond and image-potential states on Ge(100) — •Jens Kopprasch[1,2], Kristof Zielke[1,2], Cornelius Gahl[1], Christian Eickhoff[1], Jörg Schäfer[3], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Straße 2a, 12489 Berlin, Germany — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — [3]Universität Würzburg, Fakultät für Physik und Astronomie, Am Hubland, 97074 Würzburg, Germany

Germanium is a material of growing interest in semiconductor industry debatted and used for solar cells, high-power transistors, infrared optics and x-ray detectors. Ge is an indirect semiconductor with a band gap of 0.67eV at 300K. The reconstruction of Ge(100) is comparable to the Si(100) surface. However, the surface electronic structure is still under debate.
In this talk we will present bichromatic 2PPE-measurements on Ge(100). We studied the photon-energy dependence of various transitions and identified the dangling-bond states D_{up} and D_{down} as well as the first image-potential state n=1. Besides the energetics the lifetime of these states have been investigated. Furthermore we discuss hot carrier dynamics in the conduction band and the concomitant surface recombination which proceed on a picosecond timescale.

O 85.3 Thu 17:00 WIL A317

Set in time of quasiparticle decay — •Yaroslav Pavlyukh[1], Angel Rubio[2], and Jamal Berakdar[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle — [2]Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, CFM- CSIC-UPV/EHU-MPC and DIPC, Av. Tolosa 72, E-20018 San Sebastián, Spain

The initial stages of the quasiparticle decay in a Fermi liquid are governed by a time-scale distinct from the scattering rates as derived from the Fermi golden rule approach. We show that the initial decay is non-exponential and that it is determined by the zeroth spectral moment of the electron self-energy. In contrast to the imaginary part of the on-shell self-energy yielding the exponential decay, the spectral moment does not depend on the artificially introduced broadening, and, thus, can be used to characterize even very small finite system with fragmented states. We performed exact and approximate configuration interaction calculations of the spectral moments of the electron self-energy and devised a numerically simple approach for computing the spreading of quasiparticle states even for very large systems.

O 85.4 Thu 17:15 WIL A317

Unoccupied dimer-bond state at Si(100) surfaces — •Thomas Fauster[1], Shin'ichiro Tanaka[2], Katsumi Tanumira[2], Christian Eickhoff[3], Martin Teichmann[3], and Martin Weinelt[3] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]The Institute of Scientific and Industrial Research, Osaka University, 8-1 Mihogaoka, Ibaraki, Osaka 567-0047, Japan — [3]Max-Born-Institut, Max-Born-Str. 2A, D-12489 Berlin, Germany

Two-photon photoemission from Si(100) shows a pronounced resonance for the occupied dangling-bond state D_{up} at photon energies around 2.95 eV. The polarization dependence indicates an intermediate state with a wave function oriented along the dimer axis. We assign this state to the antibonding dimer-bond orbital forming a surface resonance.

The interaction of the dimer-bond state with the bulk continuum leads to a Fano-like lineshape of the resonance curve. A two-dimensional Fano model including the interaction of the D_{up} state with bulk states can describe the data very well. The lifetime of the dimer-bond state is below 5 fs. The parameters for the D_{up} state are known from the description of the resonance curve observed for image-potential resonances.

O 85.5 Thu 17:30 WIL A317

Analysis of Si(001) 2PPE spectra obtained from *ab initio* simulations — •Henning Husser and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

Two photon photoemission spectra have been calculated for the Si(001) surface by means of direct simulation of the time-dependent photocurrents. This work is motivated by experimental observations by Fauster *et al.* [1], Shudo and Munakata [2], and Kentsch *et al.* [3]. We present a series of spectra for both *s*- and *p*-polarized light and photon energies in the range of 2.8 – 4.8 eV. Time-dependent excitation spectra are derived approximately by projection of the time-dependent wavefunctions onto the Kohn-Sham eigenstates in order to investigate the dynamics of the photoemission process. The selection rules for the 2PPE process will be compared to the selection rules for 1PPE. In order to explore the possibility of surface resonances which might lead to an enhancement of the photoemission intensity in particular from the dangling bond state, we have calculated the projected density of states at the Si(001) surface in the energy range of the intermediate states.

[1] T. Fauster, S. Tanaka, K. Tanimura, Verhandl. DPG (VI) 45, 3/544 (2010). [2] K. Shudo and T. Munakata, Phys. Rev. B **63**, 125324 (2001). [3] C. Kentsch, M. Kutschera, M. Weinelt, Th. Fauster, M. Rohlfing, Phys. Rev. B **65**, 035323 (2002).

O 85.6 Thu 17:45 WIL A317

Dynamics of the intramolecular charge transfer in alkanethiolate self-assembled monolayers — Ping Kao[1], Stefan Neppl[2], Peter Feulner[2], David L. Allara[1], and •Michael Zharnikov[3] — [1]Departments of Chemistry and Material Science, Pennsylvania State University, University Park, PA 16802, USA — [2]Physik Department E20, Technische Universität München, D-85747 Garching, Germany — [3]Angewandte Physikalische Chemie, Universität Heidelberg, D-69120 Heidelberg, Germany

Charge transport (CT) in individual molecules and their functional units is important for many frontier areas of modern science and technology. In particular, little is known about CT dynamics in self-assembled monolayers which are prototypes of future molecular electronics devices. By the example of alkanethiolate films on Au(111), we show that this phenomenon can be successfully addressed by resonant Auger spectroscopy, using the core hole clock method. The CT pathway was unambiguously defined by resonant excitation of the nitrile tailgroup attached to the alkyl backbone. The length of this backbone was varied to monitor the respective dependence of the CT time. Similar to the static conductance, this dependence was found to be coarsely described by an exponential function with an attenuation factor of 0.93 per a methylene unit. As a result, the CT time is quite long even for a short alkyl chain; e.g. ca. 100 fs for the chain of only four methylene units. In contrast, the CT time associated with the thiolate headgroup anchor was found to be less than 2.3 fs, suggesting an efficient interfacial coupling between the molecular backbone and substrate.

O 85.7 Thu 18:00 WIL A317

Electron Spin Dependent Transmission through Self-assembled Monolayers of dsDNA — •Matthias Kettner[1], Benjamin Göhler[1], Daniel Nürenberg[1], Volker Hamelbeck[1], Tal Markus[2], Zeev Vager[3], Georg F. Hanne[1], Ron Naaman[2], and Helmut Zacharias[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster, Germany — [2]Department of Chemi-

cal Physics, Weizmann Institute, Rehovot, Israel — [3]Department of Particle Physics, Weizmann Institute, Rehovot, Israel

Electron spin polarization has been measured for photoelectrons emitted from a gold substrate and transmitted through a self-assembled monolayers of chiral double-stranded DNA molecules. Electron spin polarization values of up to 60% are obtained independent of the polarization of the incident light. The measured electron spin polarization shows a dependence on the thickness of the layer, tested by varying the length of the oligomers. For surfaces covered with single-stranded DNA molecules, which do not form a well ordered layer, no significant spin polarization could be observed.

Samples are irradiated by either circularly or linearly polarized 213nm laser radiation, exciting photoelectrons within the gold substrate, not being sufficient to ionize adsorbed dsDNA molecules. Photoelectrons are analysed either by a time-of-flight detector or a small size conventional Mott polarimeter for spin analysis.

O 85.8 Thu 18:15 WIL A317

Time-resolved Fermi surface mapping and dynamics of the double-CDW transition in $HoTe_3$ — •L. Rettig[1,2], R. Cortes[1,3], J.-H. Chu[4], I.R. Fisher[4], F. Schmitt[4], P.S. Kirchmann[4], Z.-X. Shen[4], M. Wolf[3], and U. Bovensiepen[2] — [1]Fachb. Physik, Freie Univ. Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Fak. f. Physik, Univ. Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany — [3]Abt. Phys. Chemie, Fritz-Haber-Institut d. MPG, Faradayweg 4-6, 14195 Berlin, Germany — [4]Geballe Lab. f. Adv. Mat. and Dep. of Appl. Phys., Stanford Univ., CA 94305, USA

The family of rare earth tritellurides RTe_3 presents a textbook-like model system to study the effects of Fermi surface (FS) nesting driven charge density wave (CDW) formation in a low-dimensional electronic system. Depending on R, the system exhibits one or two successive CDW transitions. The collective excitations responsible for such phenomena can be investigated by time-resolved experiments. Employing fs time- and angle-resolved photoemission, the ultrafast melting of the CDW gapped state and the excitation of the amplitude mode could be demonstrated in the single-CDW compound $TbTe_3$. Using a novel position-sensitive Time-of-Flight spectrometer (pTOF) [2], we were now able to investigate the dynamics of both occupied and unoccupied electronic states over a contiguous area of the reciprocal space. Thus, we can follow the evolution of the FS after optical excitation with fs time resolution and observe the dynamics even of the smaller gap and its amplitude mode in the double-CDW compound $HoTe_3$.

[2] P. S. Kirchmann, et al., Appl. Phys. A 91, 211 (2008)

O 85.9 Thu 18:30 WIL A317

Electronic structure and electron dynamics on Si(001) studied by two-photon photoemission — •Christian Eickhoff[1,2] and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Straße 2a, 12489 Berlin, Germany — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany

In this talk we will give an overview on the electron dynamics at the Si(001) surface. In the first part we will present new aspects regarding the electronic structure of the silicon surface. The temperature dependent changes in the binding energies of the dangling-bond surface states D_{up} and D_{down} and of the ionization energy will be discussed. In the second part we will highlight the rich variety of carrier dynamics in the conduction band which we access in a femtosecond pump-probe photoemission experiment using an electron analyzer with 2D-CCD-detector. Starting with the relaxation of photoinduced carriers in the Γ_{15}- and X_1-valley we followed the scattering pathway of carriers to the normally unoccupied surface state D_{down}; a process also known as surface recombination. Subsequent relaxation of the electrons in the dispersing branch of the dangling-bond band D_{down} by electron-phonon scattering is slowed down when reaching the band minimum. This is attributed to the blockade of optical phonon emission close to the D_{down} band bottom.

O 85.10 Thu 18:45 WIL A317

How to do time-resolved photoelectron spectroscopy at a free-electron laser — •Christian Sohrt[1], Stefan Hellmann[1], Martin Beye[2], Timm Rohwer[1], Martin Marcynski-Bühlow[1], Matthias Kalläne[1], Florian Sorgenfrei[3], Michael Bauer[1], Alexander Föhlisch[2], Wilfried Wurth[3], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24118 Kiel, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, 12489 Berlin, Germany. — [3]Institut für Experimentalphysik and Center for Free-Electron Laser Science, Universität Hamburg, 22761 Hamburg, Germany

The Free-Electron Laser in Hamburg (FLASH) generates highly brilliant, ultrashort, and coherent pulses in the soft X-ray regime enabling many fascinating experiments that are not possible at other sources. After various challenges concerning space-charge effects as well as timing, synchronization and data aquisition issues have recently been solved, optical pump-XUV probe photoelectron spectroscopy on solid surfaces is now possible. The wide probing photon energy range of up to 1000 eV should allow time-resolved core-level spectroscopy with time and energy resolutions of ∼200 fs and ∼100 meV, respectively. We performed a proof-of-principle experiment on the correlated layer compound $1T$-TaS_2 [1] demonstrating that FLASH can indeed be used to investigate core-level dynamics at solid surfaces on the femtosecond time scale. This work is funded in part by the BMBF (FSP 301 FLASH).

[1] Hellmann *et al.*, PRL **105** 187401 (2010)