

O 12 Methods

Time: Monday 15:00–17:15

Room: WIL B321

O 12.1 Mon 15:00 WIL B321

Near-field effects in heat transfer under UHV conditions — ●ULI F.-WISCHNATH, ACHIM KITTEL, and ANDREAS KNÜBEL — Uni Oldenburg, Fak. V, C. v. Ossietzky Str., 26111 Oldenburg

The heat transfer between a sample and a probe in an STM based SThM (Scanning Thermal Microscope) is dominated by near field radiation when approaching to small separations under UHV conditions. The nature of this evanescent part of the radiation is subject to ongoing discussions, especially the dependencies on temperature difference and distance.

We have measured the heat transfer between a gold-platin thermoelement as probe and different samples. The classical theory of fluctuating charge carriers predicts a strong increase when approaching the sample. This can be observed for separations ranging from roughly 100 nm down to the order of one nanometer. For even smaller separations a nearly constant value is found showing the breakdown of the classical theory.

We were able to trace the increase of the heat transfer above the far field value up to separations of about 100 nm due to a new production process of the thermoelement. The more filigree new probe has its sensitive area about 100 times closer to the very end of the tip and has a ten times greater thermal resistance. This results in an increase in sensitivity by a factor of 15 compared to the ones used previously.

O 12.2 Mon 15:15 WIL B321

Characterization of a time-of-flight spectrometer using photoemission with higher harmonic radiation — ●ANDREA MELZER, ALVARO WULFF, JINXIONG WANG, and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

By focussing laser pulses with 1.4 mJ energy, 30 fs pulse length and 779 nm wavelength from a multipass amplifier at a repetition rate of 1 kHz into argon photon energies up to 52 eV are generated. A grating monochromator with two interchangeable toroidal gratings (250 and 950 lines/mm) is used to select individual harmonics. A time-of-flight spectrometer for electrons is designed with a large detection angle of 34°. A fast detection electronics is used with a time-resolution of 200 picoseconds to obtain an energy resolution in the meV range. A Cu(111) surface was used to characterize the time-of-flight spectrometer and the results are compared to data obtained on the same surface with a hemispherical energy analyzer.

O 12.3 Mon 15:30 WIL B321

Improvement of temporal resolution on Ultrafast Electron Diffraction (UED) experiments — ●MATTHIAS WIELENS, ANJA HANISCH, BORIS KRENZER, and MICHAEL HORN-VON HOEGEN — Universität Duisburg-Essen, Institut für Experimentelle Physik, Lotharstrasse 1, 47057 Duisburg

For Ultrafast Electron Diffraction experiments studying transient phenomena at surfaces and in bulks upon laser excitation a high temporal resolution is essential. In our surface sensitive Reflection High Energy Electron Diffraction setup the resolution is limited by the so called “*velocity mismatch*” between the velocity of light and the much lower velocity of high energy electrons. Due to their grazing incidence the electron pulse needs a few 10 ps to travel across the sample. The excitation by the fs laser pulses at normal incidence with the pulse front parallel to the surface, however, occurs instantaneously. Thus, temporal overlap is not given. In consequence, this leads to an averaging of the observation of transient phenomena during the time the electron pulse probes the sample.

A solution to this problem is to tilt the pulse front of the laser pulses with respect to the propagation direction at such an angle that ensures temporal overlap between the pulse fronts of the two beams. For 10 keV electrons with a grazing angle of incidence of 5° this requires a tilt angle of almost 80°!

We present an experimental setup that facilitates such a large tilt angles and will demonstrate the improvement in temporal resolution of our ultrafast electron diffraction setup.

O 12.4 Mon 15:45 WIL B321

How the solid state matrix affects the chemical shift of core-level binding energies: A novel method to take the induction effect into account — ●KUNYUAN GAO, THOMAS SEYLLER, and LOTHAR LEY — Institut für Physik der Kondensierten Materie, Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Erwin-Rommel-Str. 1, D-91058 Erlangen, Germany

Small binding energy variations of core levels, i.e., chemical shifts provide useful information about the chemical environment of the atom under investigation. With the widespread use of synchrotron radiation as excitation source for photoelectron spectroscopy a vastly improved spectral resolution compared to conventional laboratory sources allows the unambiguous identification of components with chemical shifts less than a tenth of an eV. As a consequence, the interpretation of the chemical shift in complex systems such as mixed oxides requires to take charge transfer beyond the first coordination shell into account. A novel scheme is presented that allows to include these so-called induction effects in estimates of chemical shifts based on the electronegativities of the constituent elements. The method is a judicious extension of Sanderson's original approach [1] towards network structures. At each point of departure from Sanderson, the method is tested successfully against the rigorous Sanderson formalism. For three crucial examples of relevance in semiconductor technology, our new method yields predictions in excellent agreement with experiment. [1] R.T. Sanderson, *Chemical Bonds and Bond Energy*, Academic Press, London, 1971, p.17.

O 12.5 Mon 16:00 WIL B321

Van der Waals Interaction: A Universal Semiempirical Supplement to DFT Tested for Various Systems — ●FRANK ORTMANN¹, WOLF G. SCHMIDT², and FRIEDHELM BECHSTEDT¹ — ¹Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany — ²Universität Paderborn, Fakultät für Naturwissenschaften, Theoretische Physik, Warburger Str. 100, 33100 Paderborn, Germany

Theoretical investigations of surface adsorbed molecules are generally carried out using Density Functional Theory within the Local Density Approximation (LDA) or the Generalized Gradient Approximation (GGA). One driving force for the adsorption process of molecules are van der Waals interactions (see [1] and [2]). Unfortunately LDA and GGA are incapable of accounting for long-range correlations for inhomogeneous systems by construction.

We supplement the DFT with a semiempirical long-range correlation term based on the London formula [3] for van der Waals interaction to cure this lack. Here we examine the transferability of the present approach to different structures and to investigate the universality with respect to the atom species under consideration.

[1] F. Ortman and W. G. Schmidt and F. Bechstedt, *Phys. Rev. Lett.* **95**, 186101 (2005)

[2] M. Preuss and W. G. Schmidt and F. Bechstedt, *Phys. Rev. Lett.* **94**, 236102 (2005)

[3] F. London, *Z. Phys. Chem. Abt. B11*, 222 (1930)

O 12.6 Mon 16:15 WIL B321

Efficiency of numerical atom-centered basis functions in all-electron electronic-structure theory: the absolute-convergence limit — ●VOLKER BLUM, JÖRG BEHLER, RALF GEHRKE, KARSTEN REUTER, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany

The most fundamental choice in practical electronic structure calculations is the underlying basis set. For structures with large empty regions (surfaces, clusters, molecules), numeric atom-centered orbitals (NAO's) are attractive [1,2]. However, the question of basis set convergence is often skirted by relying on fixed basis set libraries and error cancellation; a straightforward route to establish the basis set limit does not exist.

We here investigate the routine feasibility of meV-level *absolute* convergence in all-electron total-energy calculations with NAO basis sets (confined atomic, ionic, or hydrogen-like), using as examples small molecules and clusters (N₂, Cu₂, Cu₄, Cu₁₀). (i) We show how to establish a systematic (over-)converged NAO basis set limit. (ii) To construct minimal-sized converged basis sets, we pick individual functions one by one from large candidate function pools, using non-selfconsistent superposition po-

tentials for maximum efficiency. ~ 50 basis functions per atom are needed for meV-level convergence in each case. (iii) We find that converged basis sets are transferable to self-consistent potentials, and from one structure to another. The total energy errors from underconverged basis sets depend systematically on the interatomic distance.

[1] B. Delley, *J. Chem. Phys.* **92**, 508 (1990).

[2] J.M. Soler *et al.*, *J. Phys.: Condens. Matter* **14**, 2745 (2002)

O 12.7 Mon 16:30 WIL B321

The influence of sample properties and finite resolution on the results of surface-XPCS measurements — •ROBERT FENDT¹, CHRISTIAN GUTT², AYMERIC ROBERT³, ANDERS MADSEN³, and METIN TOLAN¹ — ¹Exp. Physik 1a, Univ. Dortmund — ²HASYLAB, Hamburg — ³ESRF, Grenoble, France

Surface-sensitive XPCS is a powerful technique for in-situ measurements on a fluctuating surface. However, recent experimental results clearly show that assuming the Fraunhofer limit (which holds in the case of PCS) is an over-simplification in the case of XPCS, yielding the need for a new theoretical treatment [1, 2]. In the case of low-viscosity liquids, which is considered here, one expects an oscillating behaviour (due to capillary waves) of the correlation function, i. e. for a homodyne setup, $G_{\text{hom}}(\vec{q}, \tau) = 1 + C \cos^2(\omega(\vec{q})\tau) \exp(-2\Gamma(\vec{q})\tau)$ with the contrast $0 < C \leq 1$. However, under special circumstances, a “heterodyne” function $G_{\text{het}}(\vec{q}, \tau) = 1 + C \cos(\omega(\vec{q})\tau) \exp(-\Gamma(\vec{q})\tau)$ is observed [3, 4]. This behaviour can be understood as a resolution effect, i. e., a finite experimental resolution $dq > 0$ enables the specular reflection from the surface to function as a static reference signal [2]. Surprisingly, recent experiments [3] suggest a possible dependence of dq on the sample material. This would essentially mean that the usual separation of specular and off-specular scattering might not be valid in the case of SXPCS.

[1] M. Sprung *et al.*: ESRF 2004, unpub.

[2] T. Gadheri: PHD thesis, to be publ.

[3] R. Fendt *et al.*: ESRF 2005, unpub.

[4] C. Gutt *et al.*: PRL 91, 076104 (2003)

O 12.8 Mon 16:45 WIL B321

An Energy Dispersive beamline for NEXAFS and other CFS/CIS studies — •D. R. BATCHELOR¹, TH. SCHMIDT¹, R. FOLLATH², CH. JUNG², R. FINK³, M. KNUPFER⁴, A. SCHÖLL¹, and E. UMBACH¹ — ¹Exp.Physik II, Univ. Würzburg — ²BESSY GmbH — ³Phys. Chem. II, Univ. Erlangen — ⁴IFW Dresden

Energy dispersive NEXAFS is a quite well known technique in the Hard X-Ray region. It is however not so well known in the Soft X-Ray region [1]. By combining the energy dispersion of a monochromator and the imaging properties of a hemispherical electron analyser the simultaneous detection of electron distribution curves as a function of photon energy is possible. The dispersion of the monochromator is projected on to the sample and subsequently imaged in the non dispersive plane of the analyser. Such an instrument is able to fully exploit the small spot size of state-of-art synchrotron monochromators and modern electron energy analysers with 2D imaging detectors. The parallel detection enables a large parameter space to be efficiently sampled such that, e.g., high energy resolution can be combined with short time scales in the ms range. We present the design for an upgrade of an existing beamline and a pilot experiment utilising the low angular divergence of a PGM which is operated at low C_{ff} values. The advantages and need for such an experimental setup will be illustrated using traditional CFS/CIS data of organic thin films.

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[1] K. Amemiya, H. Kondoh, T. Yokoyama, T. Ohta, *Journal of Electron Spectroscopy and Related Phenomena* 124 (2002) 151 – 164

O 12.9 Mon 17:00 WIL B321

New potentialities at the ESRF surface diffraction beamline ID03 — •N.M. JEUTTER, I. POPA, D. WERMEILLE, H. ISERN-HERREA, E. PAISER, L. PETIT, T. DUFRANE, and R. FELICI — ESRF, 6 Rue Jules Horowitz, 38000 Grenoble, France

The ESRF surface diffraction beamline ID03 has been devoted to structural and dynamical studies of surfaces and interfaces since 1993. Structural and dynamical studies like epitaxial growth, surface kinetics and phase transitions resulted in many publications. The hutch 1 diffractometer can host small UHV, catalysis and electrochemistry cells. In the hutch 2 the diffractometer coupled with a large UHV chamber, allows the studying of the structures and the kinetics of adsorbates or homostruc-

tures. A refurbishment program is currently underway. An upgrade of the monochromator takes place in order use the full brightness of the undulator source, and to allow for an easier control on the selected used beam energy. The optics of the beamline will be improved in order to achieve a focussing at the sample of the order of few squared microns. The modernisation of the experimental hutch 2 will allow users to install their own UHV systems and will simplify the changing of the samples on the provided chamber. Aim of this contribution is to show to the surface science community the status of the ID03 refurbishment plan and the new opportunities provided by the upgraded instrumentation.