

ÉCOLE DE PHYSIQUE  
LES HOUCHES



# SUCCESS 2014

School on UV and X-ray Spectroscopies of Correlated Electron Systems

*Ecole de Physique des Houches, France*

*1-12 September 2014*

Organized by

Andres Santander-Syro

Patrick Le Fèvre

Ralph Claessen & Friedrich Reinert



Administration: Iskouhie Métérien (Synchrotron SOLEIL)

Sponsored by





	Mon 1/9	Tue 2/9	Wed 3/9	Thu 4/9	Fr 5/9	Sat 6/9	Sun 7/9	Mon 8/9	Tue 9/9	Wed 10/9	Thu 11/9	Fr 12/9
7h45 8h45		Brkfst	Brkfst	Brkfst	Brkfst	Brkfst	Brkfst	Brkfst	Brkfst	Brkfst	Brkfst	Brkfst
8h45 10h15		Intro 15 min PES-EXP-1 Claessen	PES-EXP-2 Claessen	PES-TH-2 Minar	PES-EXP-3 Claessen	Novel Analyzers-1 Schönhense		XRS-1 X-RS Abbamonte	XRS-3 X-RS Abbamonte	HAXPES-1 Fadley	TR-PES-2 Perfetti	STUDENTS' TALKS 8:45 – 10:00
10h15 10h45		Coffee	Coffee	Coffee	Coffee	Coffee	Free	Coffee	Coffee	Coffee	Coffee	Coffee 10:00 – 10:15
10h45 12h15		PES-TH-1 Minar	SCES-1 Biermann	SCES-2 Biermann	Tutorial SPR- KKR package Minar	Novel Analyzers-2 Schönhense		XRS-2 RIXS Monney	XRS-4 RIXS Monney	HAXPES-2 Fadley	ARPES- Orbital Tomography Reinert	STUDENTS' TALKS 10:15 – 11:05 Closing 30min
12h30 14h00		Lunch	Lunch	Lunch	Lunch	Lunch	Lunch	Lunch	Lunch	Lunch	Lunch	Lunch
14h00 16h00		Free	Free	Free	Free	Free	Free	Free	Free	Free	Free	Free
16h00 17h30		Light-Src-1 Synchrotron Couprie	Light-Src-2 Synchrotron Couprie	SCES-3 Biermann	SCES-3 Biermann	STUDENTS' TALKS 16:00 – 17:15 Coffee 17:15-17:45		HR-ARPES- 1 Santander- Syro	Spin- ARPES 1 Bertran	TR-PES-1 Perfetti		
17h30 17h45	Arrival	Coffee	Coffee	Free	Coffee 17:30 – 18:00	STUDENTS' TALKS 17:45 – 19:00	Free	Coffee	Coffee	Coffee	Free	Free
17h45 19h15		XPS-SCES-1 Haverkort	XPS-SCES-2 Haverkort 19h00 Pot d'accueil		STUDENTS' TALKS 18:00 – 19:15			HR-ARPES- 2 Santander- Syro	Spin- ARPES 2 Bertran	State of the art ARPES instrumentation Dedkov (SPECS)		Departure
19h30 21h00	Dinner	Dinner	Dinner	Dinner	Dinner	Dinner	Dinner	Dinner	Dinner	Dinner	Dinner	Dinner
21h00-						POSTERS + snacks/drinks				POSTERS + snacks/drinks		

**Photoemission Basics: EXperiment, Theory, SCES(Exp/Theo)**

Novel electron and spin analyzers

High Resolution (HR) ARPES

State-of-the-art ARPES: analyzers, detectors and excitation sources

Light sources and Synchrotron Radiation

Core-level spectroscopy of SCES X-Ray scattering (XRS): RIXS, REXS, XAS, etc

Spin-ARPES (SARPES) Soft & Hard X-ray PES

Time-resolved ARPES ARPES: orbital tomography

# Lectures

# Photoelectron spectroscopy: The joys and pitfalls of the photoelectric effect

Ralph Claessen

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Photoelectron spectroscopy (PES) in its many variants is the most direct and powerful experimental tool to probe the microscopic electronic structure of condensed matter. Although its basic principles can be readily understood from the physics of the photoelectric effect, a number of assumptions and approximations are involved, before a PES signal can be converted into useful information. Assuming that the attendants of the School have already some basic knowledge of the method (as practitioner or as theorist), my introductory lectures will try to provide an overview of the central concepts and ideas underlying the PES methodology and prepare the grounds for the subsequent SUCCESS lecture program. Besides the obvious essentials I will also try to touch upon some special issues, which are not treated often in the standard literature but may become relevant as the technique progresses into novel regimes of photon intensity and/or energy. Among the topics I plan to cover are (not necessarily in this order and time permitting):

- PES instrumentation: past, present, future
- Fermi's Golden Rule and the dipole approximation
- Photoemission final states and the  $k_{\perp}$  problem
- Surface photoemission: the  $\text{div } \vec{A}$  term
- Many-body theory of PES: Sudden Approximation and Spectral Function
- Momentum and angular information in ARPES vs. XPS: the Debye Waller factor
- Resonant photoemission: quantum interference at work

The focus of my lectures will be on the conceptual physics, with more room for comprehensive theory and detailed research examples left to the following, more specialized lectures.

## Theoretical description of ARPES: one step model of photoemission

Jan Minar

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Spectroscopy is an extremely important experimental tool providing information on the electronic structure of the probed system that has to be seen as a stringent benchmark for the success of any electron structure theory. Photoemission spectroscopy (PES) or its inverse – the Bremsstrahlen isochromat spectroscopy (BIS) – in their angle-integrated form should reflect the density of states (DOS) rather directly, in particular in the high photon energy regime (XPS). For that reason it is quite common to check the ab-initio calculations by comparing the calculated DOS directly to PES spectra. However, this approach ignores the influence of the specific PES matrix elements that in general will introduce an element- and energy-dependent weight to the partial DOS.

In case of angle-resolved photo emission (ARPES) the situation is even more severe as the surface as well as dipole selection rules may have a very pronounced impact on the spectra demanding for a coherent description within so called one-step model of photoemission.

In the first lecture, I will present a general theoretical description of the ARPES by means of one-step model of photoemission. After the historical overview of this method, I will discuss how to solve the Fermi golden rule for semi-infinite surface. This is done by multiple scattering Greens function KKR method.

In the second lecture I will present recent developments of the one-step model of photoemission as, for example, inclusion of correlation effects by means of dynamical mean field theory (DMFT), description of disordered alloys by so called coherent potential approximation (CPA) and inclusion of electron-phonon coupling. All developments will be followed by corresponding examples covering the wide photon energy window, e.g. from laser photoemission up to soft and hard-X-ray regime.

In the third lecture I will present features of the Munich SPR-KKR package including graphical user interface xband. This package includes possibility to calculate various spectroscopic methods, in particular ARPES.

## Synchrotron radiation and FEL properties in the landscape of short wavelength sources

Marie-Emmanuelle Couprie

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More than 50 years after the lasers' discovery, VUVX light sources are actively developed around the world.

The X-ray laser and High order Harmonic Generation in Gas (HHG) or on solid targets take advantage of the light emission properties of matter. Recently, the use of single, few-cycle laser pulses in the mid-infrared enabled to provide tuneable radiation to above keV energies with a few attoseconds duration.

Synchrotron radiation is emitted by accelerated relativistic charged particles. In accelerators, it is produced when the particle trajectory is subjected to a magnetic field, either in bending magnets or in specific insertion devices (undulator) made of an alternated succession of magnets, allowing the number of curvatures to be increased and the radiation to be reinforced. After the historical remarks, the general properties of synchrotron radiation will be discussed. An example of undulator radiation is shown in Fig. 1. Synchrotron radiation is a « white» source, tuneable from infra-red to X-rays. With a low divergence and small size source, it is a brilliant source. It can provide different types of polarizations. It is a pulsed radiation, which duration results from that of the electron bunch from which it is generated. Depending on the accelerator type, it appears at a high repetition rate (typically MHz for storage rings, kHz for superconducting linear accelerators and 10-100 Hz for normal conducting linear accelerators). Technology of undulator and wiggler will also be introduced.



*Figure 1: ACO undulator radiation.*

Synchrotron radiation from third generation light sources provides presently partial transverse coherence thanks to the low value of the emittance (product of the beam size by its divergence). Quest for diffracted limited storage rings is now under way for improving the coherence. Usually, the needed spectral range is selected via a monochromator.

The longitudinal coherence is achieved by setting in phase the electrons, thanks to an energy exchange between the electrons and a light wave (the spontaneous emission or an external seed) resulting in bunching and further amplification of the light according to the Free Electron Laser process. Presently, these so-called fourth generation light sources are operating in the world for users : LCLS (Stanford, USA) and SACLA (Harima, Japan) in the 1-0.1 nm spectral range, with up to several mJ energies, FLASH (Hamburg, Germany) and FERMI (Trieste, Italy) in the XUV region, FERMI being the first seeded FEL open for users. These light sources provide short pulses, in the femtosecond range, and extremely high brilliance. Implied processes, FEL schemes and the FEL panorama will be given.

In the quest to the fifth generation of acceleration based light sources, paths towards advanced and compact FELs are open. In order to approach diffraction and Fourier limits in a wide spectral range and with versatile properties, one considers FEL oscillator in the X ray range, advanced seeding, multiple simultaneous operation, high repetition rate... In order to search for compactness, one considers investigating further the seeding schemes for the FEL line and replacing the conventional linear accelerator by a compact alternative one, such as dielectric accelerator, inverse FEL and Laser WakeField Accelerator (LWFA). Indeed, the rapidly developing LWFA are already able to generate synchrotron radiation. With an electron divergence of typically 1 mrad and an energy spread of the order of 1 %, an adequate beam manipulation through the transport to the undulator is needed for FEL amplification. Several directions are explored within the LUNEX5 (free electron Laser Using a New accelerator for the Exploitation of X-ray radiation of 5th generation) project, aiming at investigating the production of short, intense, and coherent pulses in the soft X-ray region with 400 MeV electron beam (both from a superconducting linear accelerator for high repetition rate multiple user operation and a LWFA, a single FEL line with HHG and Echo Enable Harmonic Generation seeding). A test experiment for the demonstration of FEL amplification with a LWFA is under preparation in the frame of the COXINEL ERC contract.

***Acknowledgments :***

The author would like to acknowledge the ERC support for the COXINEL Grant.

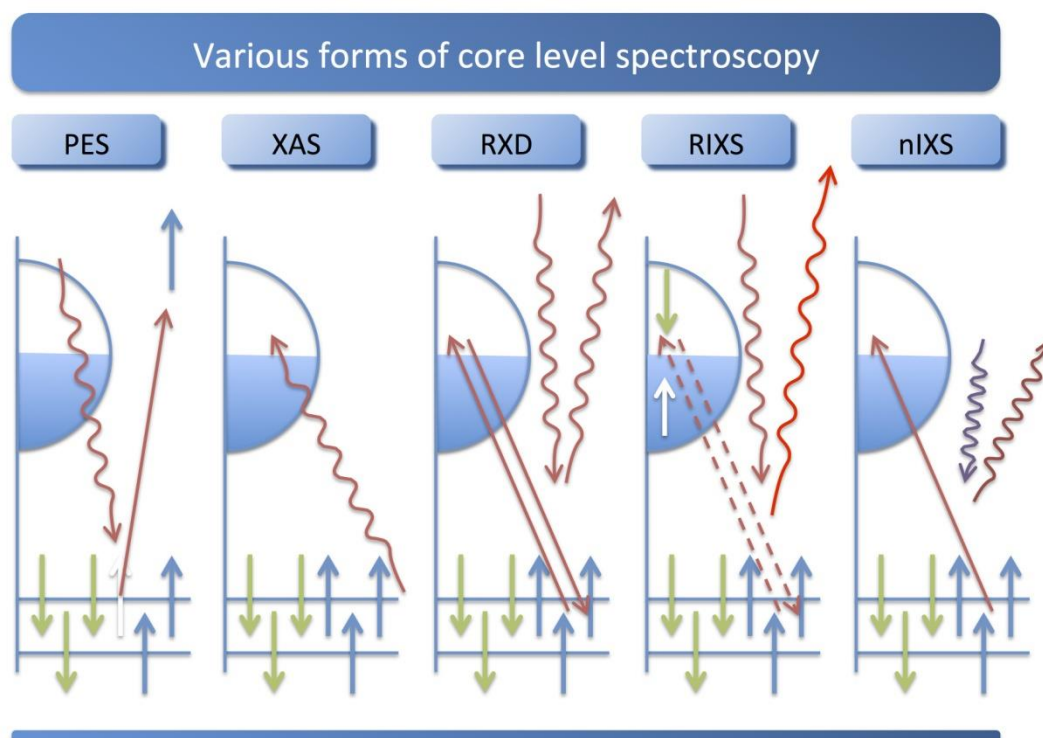


## Core level spectroscopy of TM and RE compounds

Maurits W. Haverkort

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Transition metal and rare earth compounds show a wealth of different properties. They are used as materials for energy storage (battery compounds), dyes in solar cells, elements in the read head of hard disks, high temperature superconductors, or the active centers in many of the known enzymes. The large variety of tunable properties of these materials is related to the large number of low energy degrees of freedom of the transition metal or rare earth ion. Correlations between the electrons in a solid lead to a detailed interplay between the local spin, charge, orbital and lattice degrees of freedom. The result is extremely rich physics of these open shell systems. At the same time the interplay between several low energy degrees of freedom make these materials involved to understand. Although enormous theoretical progress has been made during the last years in the understanding of correlated materials one often needs experimental input to understand particular phenomenon.



**Figure 1:** Various forms of core level spectroscopy that will be discussed during the lecture.

*PES* – (core level) photoelectron spectroscopy

*XAS* – X-ray absorption spectroscopy

*RXD* – resonant x-ray diffraction

*RIXS* – resonant inelastic x-ray diffraction

*nIXS* – (non-resonant) inelastic x-ray scattering

Core level spectroscopy in many cases turns out to be a very efficient method to study the many body properties of these systems. Core level photoelectron spectroscopy allows one to determine how the low energy Hamiltonian arises from the high-energy scale interactions. It thus provides information on the

low energy model parameters of the system. X-ray absorption spectroscopy contains information on the local electronic structure. It provides information on the symmetry of the wave function, such as the local spin-state or orbital occupation. Resonant x-ray diffraction is related to x-ray absorption, in addition to x-ray absorption it allows one to study the spatial dependence of local electronic order in the system. Resonant inelastic x-ray scattering allows one to study the dynamics of low energy excitations. Non-resonant inelastic x-ray scattering of core level excitations is a technique rather comparable to x-ray absorption spectroscopy with the difference that it allows for non-dipole transitions, useful in the study of involved orbital or multipole ordering.

For the understanding of these spectra, in this class of materials, it is important to realize that one needs to treat the interactions between the electrons beyond mean field approximations. It is not sufficient to assume independent electrons interacting with an average potential, but one has to consider the interaction between each pair of electrons explicitly. In the spectra this leads to excitons and multiplets that dominate the spectral line-shape.

In this talk I will discuss these various forms of core level spectroscopy, which material properties one can obtain with these techniques and how to theoretically understand these spectra.

**Further reading:**

*Core level spectroscopy of Solids* – Frank M. F. de Groot and Akio Kotani

*NEXAFS Spectroscopy* – Joachim Stöhr

*Introduction to ligand field theory (chapter 1-6)* – Carl Johan Ballhausen (1962)

*Physical Chemistry (chapter 13-18 (10-15) edition 5 (8))* – Peter Atkins (2006)

*Multiplet ligand-field theory using Wannier orbitals* – M. W. Haverkort, M. Zwierzycki, and O. K. Andersen (PRB 2012)

## **Strongly correlated materials**

Silke Biermann

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The field of electronic structure calculations for correlated materials has witnessed tremendous progress in recent years due to the development of combined electronic structure and many body theories. We will give an introduction to the concept of electronic correlations and the modeling thereof. Then we will give an overview of density functional theory (DFT), the workhorse of modern electronic structure calculations, and discuss some of its successes as well as failures. Having evidenced the need of going beyond DFT, we will summarize some of the main strategies of many-body theory and their combination with realistic electronic structure techniques. We will describe the ideas and formalism of dynamical mean field theory, and discuss its application in the electronic structure context. Finally, we will comment on current questions in the field and open challenges. The lectures will thus be structured as follows:

- 1) Correlation effects in condensed matter - Brief overview
- 2) Spectroscopic signatures of correlations
- 3) Modeling correlated electron behavior
- 4) Tools of many-body theory -- survival kit
- 5) Density Functional Theory (DFT) - An introduction
- 6) Successes and failures of DFT: the need of going beyond
- 7) Dynamical mean field theory
- 8) Electronic structure calculations for correlated materials: the present status
- 9) What about U?
- 10) Perspectives and open questions

# NOVEL ANALYZERS

## Concepts for a higher degree of parallelization in data acquisition: k-microscopy and parallel spin detection

Gerd Schönhense

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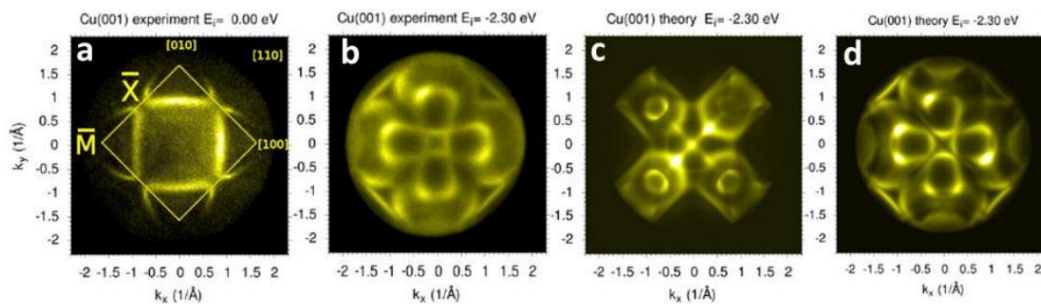
Hemispherical analyzers are the “working horses” of photoelectron spectroscopy. After half a century of development they have nowadays reached a high degree of maturity but also their principal limits. Benchmarks are sub-meV energy resolution and  $0.2^\circ$  angular resolution, thus giving access to subtle features in the band structure [1]. Inherently, these analyzers are limited in the accepted solid angle interval to several degrees, depending on the desired angular resolution. Along with an increasing demand for energy and angular resolution data-acquisition speed has become an issue, especially for reactive surfaces and – dramatically – when it comes to spin-resolved detection. This lecture will address alternative ways of photoelectron spectroscopy (spin-integral and spin-resolved) aiming at a higher degree of parallelization. Such new concepts are most important for time-resolved studies of transient states and spin-resolved spectroscopy. The low performance of present (single-channel) spin detectors is prohibitive for many experiments. As there is practically no literature yet, this abstract gives an extended introduction into the new field of k-space microscopy.

### I. Momentum microscopy

This alternative approach makes use of a basic concept of microscopy: In each imaging optical system the so-called *reciprocal* image represents the distribution of the transversal momentum components. In mathematical language we can term it the *Fourier* image, providing the distribution of “spatial frequencies” (being nothing else than the momentum pattern). Owing to  $k_{\parallel}$ -conservation in the photoemission process, the reciprocal image formed by the objective lens of a photoemission microscope directly yields the surface-projected band structure inside the crystal. This image occurs in the backfocal plane of the cathode lens [2]. In momentum microscopy this *Fourier* pattern is imaged with ultimate  $k$ -resolution. The intriguing advantage is that this method gives access to the  $k_{\parallel}$ -distribution of the full half-space above the solid. Given sufficiently high photon energy, the half space corresponds to a large momentum range exceeding the first *Brillouin* zone.

#### I.1 Using a dispersive energy filter

Implementation of an imaging dispersive analyzer allows displaying of the  $k_{\parallel}$ -distribution at a selected energy. This method was pioneered by J. Kirschner’s group at MPI Halle.



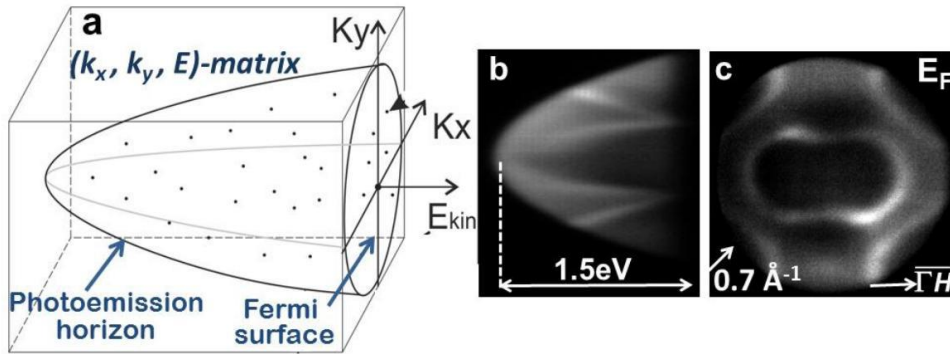
**Figure 1:** Momentum microscopy images for Cu(001) at the Fermi energy (a) and at a binding energy of 2.3 eV (b) in comparison with a calculation without (c) and with self-energy correction (d). (from [4])

Impressive  $k$ -patterns have been measured, e.g., for Cu [3,4]. A typical result for the Cu(001) surface is shown in Fig. 1. Comparison with the calculation (by J. Henk's group) reveals that a self-energy correction with parameters  $\Sigma_d = -0.8\text{eV}$  and  $\Sigma_{sp} = +0.3\text{eV}$  yields best agreement between experiment and theory (for details, see [4]). In principle,  $k_{\parallel}$ -images of the full half space at the selected energy like those in Fig.1 can be observed on the fluorescence screen of the momentum microscope with the bare eye in real time (provided the photon flux is sufficiently high). 2D  $k_{\parallel}$ -distributions at different energies are acquired sequentially.

### 1.2 Implementing time-of-flight (ToF) parallel energy detection

Going further in parallelization, we are developing a 3D-method for  $k$ -space mapping with utmost efficiency by implementing an imaging time-of-flight ToF spectrometer instead of the dispersive (i.e. bandpass-type) spectrometer. This approach adopts the concept of ToF-PEEM [5,6], the heart of the experiment being a 3D  $(k_x, k_y, t)$ -resolving image detector (delay-line detector [7,8] with 150ps time resolution and 10Mcps maximum count rate). This approach requires pulsed photon sources like synchrotron radiation, lasers or higher-harmonic sources. Fig. 2 illustrates the principle: All counting events in the  $E$ - $k_{\parallel}$  paraboloid confined by the Fermi-energy cut and the photoemission horizon (condition  $k_{\perp}=0$ ) are detected at fixed setting of the  $k$ -microscope. The binding energy (with respect to  $E_F$ ) is determined as in classical photoemission ( $E_B = h\nu - E_{kin} - \Phi$ ;  $\Phi$  workfunction) utilizing the relation  $E_{kin} \propto \text{ToF}^2$ . The software of the delay-line detector accumulates the counting events in the  $(k_x, k_y, E_B)$ -voxels of the data matrix. For visualization, sections can be made in every plane (or 3D tomograms).

**Figure 2:** 3D acquisition principle of a ToF  $k$ -microscope. Schematic view of the  $(k_x, k_y, E_B)$  data matrix acquired



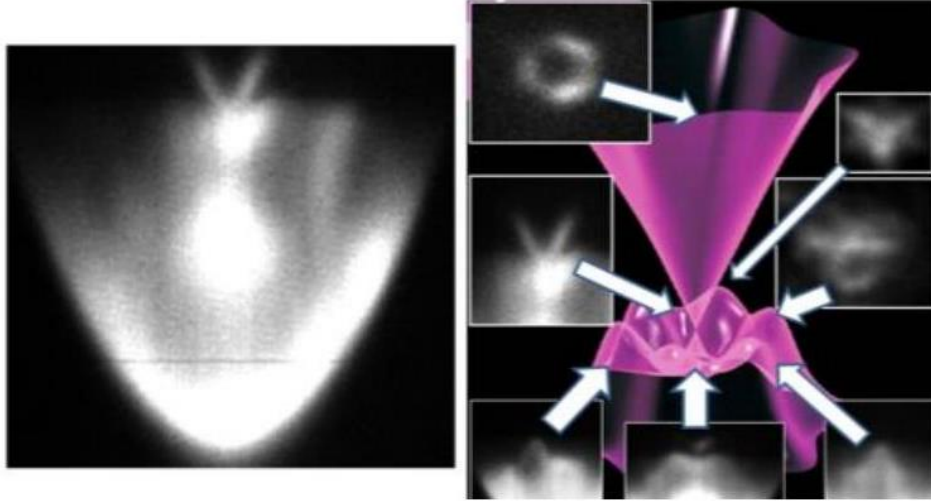
simultaneously (a). The  $k$ -space sections show the bands in an  $E$ - $k_{\parallel}$  plane (b) and a cut through the Fermi surface (c) of Mo(110), taken with 2PPE excitation by 3.3eV photons from a TiSa laser.

As test case for the performance we have chosen the topological insulator  $\text{Bi}_2\text{Te}_3$ , because detailed data with conventional high-resolution ARPES spectrometers exist [10]. Fig. 3 shows a collection of sections through several planes in the vicinity of the Dirac cone. Note that Fig. 3 shows the raw data without any treatment (like symmetrization) and the 3D data matrix has been taken in a few minutes of total acquisition time.

### 1.3 What can be gained by this novel approach?

In the first experiments a frequency-doubled Ti-sapphire laser was used for 2PPE excitation at  $2h\nu = 5.8$ – $6.6\text{eV}$ . Mapping a complete data set with good statistics requires only few minutes of acquisition time; Fig. 2b,c shows an example taken for the Mo(110) surface. In a first experiment with Synchrotron radiation ( $h\nu = 35\text{eV}$ ) at BESSY (Berlin) a much larger energy-and  $k_{\parallel}$ -range became accessible. Under non-optimal

conditions of this first run energy- and  $k$ -resolution were about 30meV and  $2 \cdot 10^{-2} \text{\AA}^{-1}$ , respectively (leaving space for improvement).



**Figure 3:** Result of a test run on a sample of the topological insulator  $\text{Bi}_2\text{Te}_3$  (sample courtesy R. Claessen and M. Scholz). Many details of the Dirac state are resolved in this run of only 5 minutes total acquisition time. The figure shows the raw data taken at room temperature.

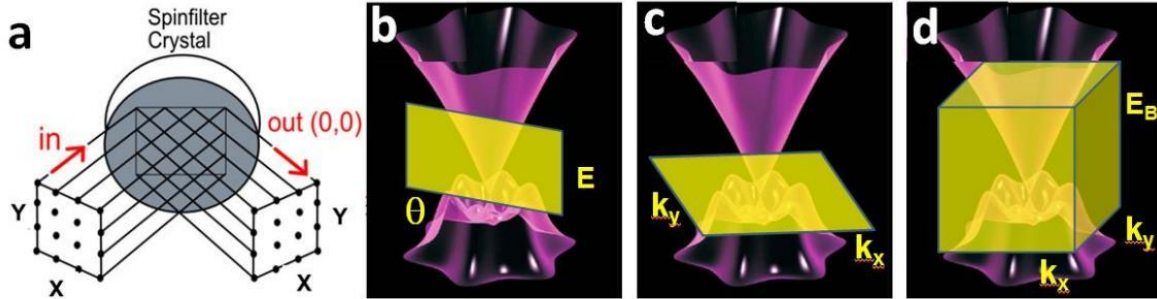
Assuming an energy interval of width 1.5eV and an observed  $k_{\parallel}$ -range of radius  $1 \text{\AA}^{-1}$  we arrive at a total number of 2,400 resolved  $k$ -points x 50 resolved energy intervals = 120,000 voxels acquired simultaneously. Under optimized conditions, more than 5,000  $k$ -points can be resolved with this kind of electron optics [9]. The ToF method is expected to reach an energy resolution in the few-meV range. This will drive the degree of parallelization towards the order of  $10^6$  voxels.

## II. Parallel spin detection

The basics of electron spin detection will be addressed in lecture [11], so here we will focus on the aspect of parallelization. Although they have reached good overall performance and ability for vectorial analysis [12], the basic concept of present spin polarimeters is not compatible with parallel detection. Recent developments towards parallel spin detection in combination with a hemispherical analyzer [13] and with an emission electron microscope [14] exploit the fact that in low-energy electron diffraction  $k_{\parallel}$  is conserved, similar to an optical mirror, as illustrated in Fig.4a. With Ir(001) [15] and Ir(001)-Au(1x1) [16] spin-filter surfaces with high figure of merit and long lifetime in UHV have been found. For high-Z materials the diffraction process is highly spin selective, usable maxima of the spin asymmetry function reach 82%.

Implementation in a hemispherical analyzer constitutes *multichannel spin detection* as demonstrated in [13] with about  $10^3$  (E,  $\theta$ ) data points acquired simultaneously, schematized in Fig.4b. The high data acquisition speed made it possible to prove half metallicity in the Heusler compound  $\text{Co}_2\text{MnSi}$  [17], being hardly possible with a common single-channel spin detector due to the fast contamination of this reactive surface. Parallel acquisition of more data points has been achieved by integrating a *spin-polarizing electron mirror in an emission microscope* with dispersive energy filter [14], in the present stage of development yielding almost  $10^4$  ( $k_x, k_y$ ) data points in parallel [9], cf. Fig. 4c. Sequential acquisition of  $k_{\parallel}$ -distributions at many energies yields the complete spin-resolved valence band structure.

Finally, *ToF k-microscopy with imaging spin filter* allows for parallel detection of the energy coordinate (via the time of flight) and thus adds the third dimension in parallel data acquisition, cf. Fig. 4d. This new approach requires solving several problems like the energy-dependence of the spin asymmetry or the chromatic aberration of the electron-optical system. The status of all three modes of parallel spin detection will be reported.



**Figure 4:** Basic scheme of parallel spin-polarization detection utilizing specular diffraction from a high-Z spinfilter crystal (a) and the application modes in combination with a hemispherical analyzer (b), *k*-microscope with dispersive energy filter (c) and *k*-microscope with time-of-flight detection (d).

**References:**

[1] cf. lectures of R. Claessen, A.F. Santander-Syro and T. Kampen.  
 [2] E. Bauer, Rep. Prog. Phys. **57** (1994) 895.  
 [3] A. Winkelmann et al., PRB **86** (2012) 085427.  
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 [5] G. Schönhense et al., Surf. Sci. **480** (2001) 180.  
 [6] A. Oelsner et al., Rev.Sci. Instrum. **72** (2001) 3968.  
 [7] A. Oelsner et al., JESRP **178-179** (2010) 317.  
 [8] <http://www.surface-concept.com>  
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 [10] S. Souma et al., PRL **106** (2011) 216803.  
 [11] for details, cf. lecture of F. Bertran.  
 [12] F. Meier et al., PRB **77** (2008) 165431.  
 [13] M. Kolbe et al., PRL **107** (2011) 207601.  
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 [17] M. Jourdan et al., Nature Commun. **5** (2014) 3974.

## **Resonant inelastic X-ray scattering**

Claude Monney

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During the last ten years, resonant inelastic X-ray scattering (RIXS) has benefited from impressive technical advances, especially in the field of synchrotron radiation and x-ray optics. Nowadays it is well recognized as an x-ray spectroscopy to probe in particular correlated materials.

In this lecture, I will introduce first the basics of RIXS, with some theoretical insights on its description, and then describe the experimental side of the technique and how measurements are performed in practice. In the framework of this summer school, I will also discuss how RIXS compares to other well established spectroscopies, including angle-resolved photoemission spectroscopy.

In a second part, I will illustrate these concepts with some recent RIXS studies on correlated electron systems, exemplifying how appropriate and diverse this X-ray spectroscopy is for understanding the physics of new materials.

Finally, I will review existing and new synchrotron beamlines across the world for performing RIXS measurements.



## **High-resolution ARPES for the study of correlated-electron materials**

Andrés F. Santander-Syro

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Angle-resolved photoemission spectroscopy (ARPES) is a powerful technique to study the microscopic properties of solids. ARPES gives direct access to the band structure of a material, and provides valuable information about the many-body interactions affecting such band structure.

On the other hand, many interesting, and even open, problems in modern condensed-matter physics involve low electronic energy scales, of the order of a few meV, and temperatures of or below a few Kelvin. The experimental study of the electronic structure of these systems is best realized using (ultra-) high resolution ARPES at very low temperatures.

These lectures will introduce the basic aspects of high-resolution ARPES, from a synopsis (or recall from previous lectures) of currently used instrumentation to its application in the study of various fascinating problems of correlated-electron systems. Time permitting, topics to be discussed include:

- Brief overview of many-body effects and how to study them using ARPES.
- Electron-phonon coupling (and similar electron-boson couplings).
- Quasi-1D systems.
- Low- and high-TC superconductors.
- 2D electron gases in transition-metal oxides.
- Kondo resonance and periodic Anderson lattice.
- Heavy fermions and exotic phase transitions

## **Spin-resolved photoemission**

François BERTRAN

*SOLEIL synchrotron, L'Orme des Merisiers, Saint-Aubin BP 48, F-91192 Gif-sur-Yvette, France*

The first part of the lecture will be devoted to generalities and to the different ways to measure spin-polarization.

It will start with some basic concepts related to the spin like the spin operators, the Pauli matrices and the spin polarization.

We will see that it is not possible to measure the spin-polarization of free electrons with a Stern-Gerlach experiment.

I will present the spin-orbit interaction. The asymmetry of this interaction is at the origin of the Mott scattering involved in the Mott detectors. The functioning principle of these detectors will be presented and we will see how to practically correct instrumental asymmetries and what are the quantities to maximize in order to improve their efficiency.

We will see that there are two other ways to measure the spin-polarization: the Polarized Low-Energy Electron Diffraction (PLEED) which is also based on the spin-orbit interaction asymmetry and the Very-Low-Energy Electron Diffraction (VLEED) which is rather based on the exchange interaction.

In the second part of the lecture we will review different physical origins of spin-polarization in photoemission on non-magnetic and magnetic materials. Different examples will illustrate the different cases.

# Application of soft- and hard- x-ray photoemission spectroscopy to the study of strongly-correlated-electron materials

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In these lectures, I will consider several recent developments in the use of soft-x-ray photoemission (XPS, SXPS) and hard-x-ray photoemission (HXPS, HAXPES, HIKE) for the study of strongly correlated and magnetic materials and their nanostructures, using recent publications from our group [1-17] and others as illustrations. These involve combined SXPS and HXPS studies of buried layers and interfaces in transition-metal oxide and magnetic multilayers [5,6,8,10,12], hard x-ray photoemission studies of the bulk electronic structure of some spintronic materials [4,7,11,14]; band-offset measurements in oxide and semiconductor multilayers [12]; the use of standing waves and/or resonant excitation from multilayer samples to enhance depth contrast in spectroscopy [1,5(a),6,10,15,16], as well as in angle-resolved photoemission (SWARPES) [1,5(b),17] and photoelectron microscopy [3]. The extension to the hard x-ray regime of ARPES (HARPES) [9,14,16], as well as of x-ray photoelectron diffraction (HXPD) [2] will also be discussed. Such combined SXPS and HXPS studies, including standing-wave excitation, have for example, permitted directly observing the depth profile of magnetization at the Fe/MgO interface [6], changes in the bonding and the k-resolved electronic structure near a buried SrTiO<sub>3</sub>/La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> interface [5], and a two-dimensional electron gas at the SrTiO<sub>3</sub>/GdTiO<sub>3</sub> interface [17].

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# Dynamics of electronic states and ordered phases in many-body systems

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## I. Visualization of electronic states far from equilibrium conditions: a survey on the time resolved photoemission approach

The recent developments of femtosecond photon sources in the ultraviolet spectral range have largely enriched the methods to probe condensed matter on ultrafast timescales. Among the possible approaches, time resolved photoemission spectroscopy displays an increasing recognition because of the unique capability to visualize the temporal evolution of electronic states. I will review the basic principles of this experimental method and discuss the most relevant results that have been published in the recent years. The seminar will introduce in a pedagogical way the dynamics of coherent phonon generation [1] and of the electronic thermalization [2]. In a second time, I will explain the physics of systems where many-body interactions are strong enough to induce a phase transition towards an order state. The brief overview of Mott insulators [3], charge density waves [4] and superconductors [5] will elucidate the mechanism leading to the broken symmetry in each case. Due the complexity of these problems, the evolution of the electronic states provides new and essential insights to the interplay among different many-body interactions. Future perspectives in this research field will be briefly discussed.

## II. Dynamics of ordering parameters in phases with broken symmetry: new insights from time resolved X-rays

Beside time resolved photoemission, several other experimental techniques are nowadays capable of tracking the properties of condensed matter far from equilibrium. In particular, the order parameter of charge ordered and magnetic phases lead to measurable signature in the Soft-X-ray absorption and X-ray scattering. Recently, the possibility to perform these experiments in a time resolved scheme allowed to monitor the collapse and revival of phases with broken symmetry. I will discuss in detail the ultrafast demagnetization and all-optical magnetic switching that occurs in transition metal compounds [6,7]. Time resolved circular dichroism is a pivotal experiment to understand the underlying mechanisms leading to such dynamical transitions. In addition, I will present pioneering X-ray scattering experiments aiming to the time resolved observation of magnetic, orbital and charge ordering states. Due to the standing progress of Free-Electron technology, this kind of experiments will have a bright future in the incoming years.

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# Orbital Tomography: Photoemission Cross-Section for the Insight into Molecules

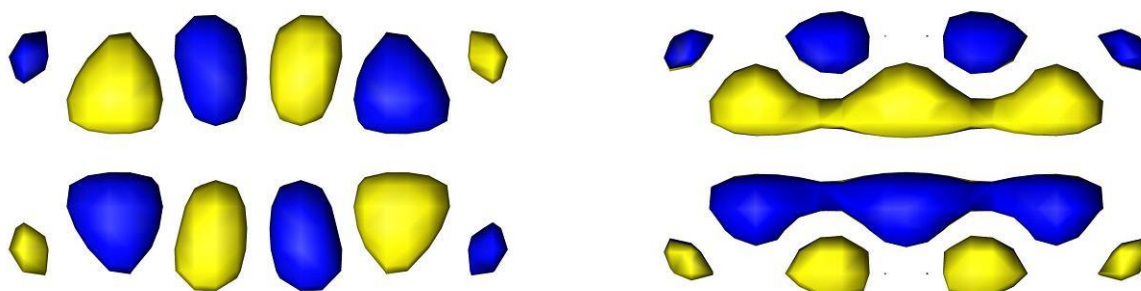
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ARPES is typically used for the investigation of the electronic band structure of solids, namely by the analysis how binding energies depend on the emission angle and the photon energy. Whereas here a strong change of the photoemission cross-section usually hinders the mapping of the band structure, the dependence of the intensity on angle and photon energy can deliver important information about the system under investigation.

Recently, it has been demonstrated [1] that the analysis of the ARPES intensity from organic molecules, adsorbed on suitable single-crystalline substrates, gives insight into the spatial structure of the valence states, i.e. the molecular "orbitals" (see Fig. 1). This *ansatz* is actually based on a simple Fourier transform of the photoemission signal from momentum space to real space, as it can be understood when one assumes a plane-wave finalstate in the photoemission process. Furthermore, circular dichroism effects [3] can possibly resolve even the symmetry of the wave-function.

In this presentation, the basic concepts of the "orbital tomography" [2] will be discussed based on the fundamental principles of photoemission theory and recent applications will be presented.



**Figure 1:** Experimental results for the *xy*-plane view of HOMO (left) and LUMO (right) of the organic molecule PTCDA on Ag(110), based on the analysis of ARPES intensities and their circular dichroism.

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## Students poster contributions

## Core-level photoemission study for 3d systems by means of dynamical mean-field approach

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Core-level X-ray photoemission spectroscopy (XPS) is a powerful tool to investigate electronic structures of strongly correlated electron systems, such as 3d-systems. Owing to recent experimental progresses, especially in bulk sensitivity and energy resolution, characteristic spectral fine features have become observed in main-line (ML) structures of  $2p$ XPS for typical transition-metal oxides (TMO)[1,2], which provide valuable information on valence electronic states (VES) near the Fermi level. As a famous example, a double-peak structure in the ML of Ni  $2p$ XPS for NiO reflects the VES related with the insulating property of NiO. [1, 3] However, a conventional theoretical framework using a single impurity model has become inadequate to extract VES information from such spectral fine structures, because many-body states in crystal, including a long-range ordering, cannot be appropriately described by the simplified framework.

In this context, recently we proposed a new framework based on the dynamical mean-field theory (DMFT) considering realistic crystal structures, which is the first attempt in this research field. [3] In our framework, the many-body states beyond the conventional SIM description are appropriately renormalized into the optimized impurity Anderson model. [3] In this talk, we report the analysis of the double-peak structure for NiO [3] and the carrier-doping dependence of the ML structure of Cu  $2p$ XPS for high- $T_c$  cuprates. We show the ML fine structures are closely related with the VES and the magnetic state near the Fermi level of NiO and cuprates. Furthermore, we will show a systematic analysis of ML structures in the series of TMO in connection with the valence electronic structure near the Fermi level.

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## Surface Properties of SmB<sub>6</sub> Studied by X-Ray Spectroscopy

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SmB<sub>6</sub> was the first example of a mixed valence compound and has been well known for its anomalous low temperature resistivity behavior for decades: At temperatures below 50 K, SmB<sub>6</sub> transmutes from a metal to an insulator but shows residual resistivity for temperatures less than 5K. Renewed interest in the mixed valent insulator SmB<sub>6</sub> comes from theoretical proposals, predicting topological protected surface states making this compound the prime candidate for the new material class of “Topological Kondo Insulators”. Indeed, elaborate transport experiments have evidenced that the residual conductivity occurs only at the surface. Although extensive experimental work has recently been done, the direct observation of the chiral spin texture of the Dirac cones, which would be the positive proof of the predicted topological protected in-gap states, is still lacking. Furthermore, it is generally well known that the surface of f-systems undergoes valence changes and reconstructions, which may also influence the properties of this material and could even form the basis of alternative scenarios generating surface conductivity. However, the nature of the surface conductivity is still elusive. Applying surface sensitive soft x-ray photoemission spectroscopy, we have investigated the surface properties of freshly cleaved SmB<sub>6</sub> single crystals at 15K monitoring the Sm valance, the chemical state of boron as well as the surface stoichiometry, and also the development of these over time and with increased temperature: We have found that the surface shows an unexpected complexity originating from both intrinsic and extrinsic changes.

## Adsorption of Glutamic acid at Ag and TiO<sub>2</sub> surfaces: understanding the bio-interface at the nanoscopic level

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The understanding of the interactions between biomolecules and metal/oxide surfaces is mandatory for all those applications in which this interaction wants to be either exploited (biomaterials, nanoelectronics, hybrid material design) or avoided (fouling, hygiene). In this frame, amino acids (AA) have a key role since they are the basic constituents of peptides and proteins and are simple enough to bring information on the chemical interaction of some biological functions with the surface. They are therefore among the most used molecules in fundamental studies.

During my Masters and PhD thesis, I participated to experiments investigating the adsorption of Glutamic acid on Ag low Miller index surfaces and on rutile TiO<sub>2</sub>(110) in the temperature range from 250 K to 400 K and with a variety of experimental techniques (photoemission, absorption and vibrational spectroscopy, scanning tunnelling microscopy).

On Ag (100), the amino acid layer was produced both by traditional effusive evaporation by a crucible and by supersonic molecular beam deposition (SMB). The latter technique consists in seeding the Glu vapour in a stream of inert carrier gas within a supersonic molecular beam source. The molecules that arrive on the surface are hyperthermal and with high degree of directionality.

Here I will compare:

(1) The results obtained on the metal and oxide surfaces by effusive deposition, with particular attention to the chemical state of the adsorbed molecules. Indeed, on Ag faces Glu molecules self-assemble in different geometries but always in the non-zwitterionic form [1-4], at variance with the majority of cases reported in literature and with what expected for analogy with other AA adsorbed on Ag(111) [5]. On TiO<sub>2</sub>, on the contrary, we found evidence of both non-zwitterionic and zwitterionic adsorption. Furthermore, a new adsorption state, characterised by a lower binding energy of the N1s level, is populated for the oxygen depleted TiO<sub>2</sub> sample, to suggest a preferential role of defect - O-vacancies in particular - in the molecule-surface interaction.

(2) The self-assembly structures produced following the different deposition methods.

# Multichannel-Spin-Polarimetry for the Analysis of Spin-Transport in Metal-Organic Interfaces

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The spin-resolved analysis of electronic properties of hybrid metal-organic interfaces is of great interest. Metal-organic materials are promising candidates for spintronic applications because of their advantageous properties and chemical flexibility. Over the past decades, the various forms of photoemission experiments have become one of the standard measurement techniques in surface physics. In contrast to conventional photon optics, an effective spin polarisation analysis of a given electron beam is difficult. Since organic materials also tend to degrade within a short period, a massive reduction of spin-resolved data acquisition time is crucial. The recently developed multichannel spin- and angle-resolved photoemission spectroscopy[1] solves this issue by enhancing the figure of merit by several orders of magnitudes, making the analysis of spin-transport (e.g. spin diffusion length) in metal-organic interfaces possible. Both, the analysis of the novel measurement technique and metal-organic interfaces will lead to new insights and prospects. Funded by Stiftung Rheinland Pfalz für Innovation (project 1038)

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## The Electronic Structure of Perfluorodecalin studied by Soft X-ray Spectroscopy and Electronic Structure Calculations

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Perfluorocarbons are a special family of molecules, which rarely exist in nature due to the high energy required to build the carbon-fluorine bond. The strong electronegative effect of fluorine on neighboring atoms is still awaiting a clear electronic structure picture description and the insight to be gained is proposed to be the origin of the unique functionalities of perfluorocarbon systems. In this work, fluorine and carbon K absorption and emission spectra of liquid perfluorodecalin are presented and analyzed in terms of density functional calculations/configuration interaction. A comprehensive view of the electronic structure is given and site-specific intramolecular interactions are investigated in detail. It is found that, while the outer fluorine atoms have excess charge in the ground state, the lowest excitations must be associated with charge transfer towards the inner carbon atoms.

## The Jahn-Teller effect in systems with strong on-site spin-orbit coupling

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It is well established that in the oxides with partly filled  $5d$  shells, such as iridates, the on-site (relativistic) spin-orbit coupling is far larger than in the  $3d$  systems and therefore cannot be neglected anymore [1]. However, unlike in the  $3d$  case, so far the electron-phonon coupling has not been included in the studies of these systems. We show that even relatively weak electron-phonon coupling may lead to qualitatively different physics of the  $5d$  oxides than the one discussed so far. Thus, we derive the effective interaction between the  $j$  'spin-orbit' coupled isospins which follows from the orbital-only interaction induced by the cooperative Jahn-Teller effect. Next, we show that such interaction may, *inter alia*, lead to a novel type of propagation of the  $j = 3/2$  spin-orbit exciton in the ordered  $j = 1/2$  antiferromagnet which, unlike in the pure superexchange model, does not require coupling to the  $j = 1/2$  'magnon' excitations [2].

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# Bi thin films on InAs(111): new electron states close to the M point.

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The Bi(111) surface is a prototype system to study Rashba splitted surface states [1]. Theoretical studies [2] predicted non-trivial topological surface states appearing on single bi-layer of Bi(111) and a more complex behaviour was suggested for a variable film thickness as a function of layer thickness [3]. This clearly indicates that the electronic properties of thin films of this material are far from being understood. The Bi(111) film actually represents a special interesting class of films having an intermediate inter- bi-layer coupling strength that may have a significant influence on the topological property.

As reported in the literature, Bi thin films are grown almost exclusively on Si(111), see e.g. [4], [5]. Here we present combined theoretical and ARPES studies of the electronic structure of Bi(111) films grown on an alternative substrate, InAs(111) . Bi growth is epitaxial and a Bi monocrystal of very high quality is obtained after depositing several monolayers. For film thicknesses  $> 10$  bi-layers a  $6 \times 1$  reconstruction appears in the LEED patterns. The reconstruction results in a new set of unexpected surface states close to the M point coexisting with the pristine Bi(111) electronic structure. We show that a proper description of the photoemission process is necessary to understand a majority of these new states. They correspond to novel bulk-like features observed close to the M point. These effects are included in the one-step model of photoemission implemented in the SPR-KKR package [6].

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# Time-resolved Auger electron spectroscopy

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We present a theory of time-resolved Auger electron spectroscopy (AES) for strongly correlated many-body systems. AES produces two conduction-band holes which are described within the framework of the Hubbard model, extended by core states to account for the dynamics of core-hole screening. We work with numerically exact states and combine several techniques: the kernel polynomial method (KPM), the commutator-free exponential time-propagation (CFET) and a mapping of the continuum states on a semi-infinite chain using orthogonal polynomials.

Points of interest (now carried over into a time-dependent framework) include the understanding of correlation-induced satellites, screening effects, the validity of a two-step description and the effects resulting from a non-perturbative treatment of the Auger process. Finally, we propose a pump-probe setup, whereby a second pulse hitting the conduction band within the core-hole lifetime allows one to measure correlation effects on that very timescale.



# Growth of potential oxide topological insulator $\text{BaBiO}_3$ by pulsed laser deposition

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Recently,  $\text{BaBiO}_3$  (BBO) has been predicted to be a possible candidate for a large gap topological insulator. However the calculations show that the protected surface states are located 2 eV above the Fermi level. To populate these states heavy electron doping is necessary. Conceivable ways to achieve such a doping are for example, the deposition of alkali metal atoms or electrostatic doping of thin BBO films by applying a gate voltage.

As a first step we have been able to deposit undoped BBO on Nb-doped  $\text{SrTiO}_3$  (STO) by pulsed laser deposition. High energy electron diffraction (RHEED) during growth shows an island-like growth mode after formation of a wetting layer on the STO substrate, which may be due to the large lattice misfit of BBO and STO. A clear LEED pattern and X-ray diffraction evidence the epitaxial growth of crystalline BBO films. Photoemission data of these films show very similar valence band structures compared to published data on undoped single crystals. Further experiments will show the feasibility of doping electrons into these samples.

## Charge carrier localization in (DOEO)<sub>4</sub>[HgBr<sub>4</sub>]·TCE and Peierls transition in TTF-TCNQ single crystals by temperature-dependent NEXAFS and HAXPES

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We investigate single crystals of (DOEO)<sub>4</sub>[HgBr<sub>4</sub>]·TCE and TTF-TCNQ as well as thin films based on triangulene derivatives and F4-TCNQ using synchrotron techniques like near-edge X-ray adsorption fine structure (NEXAFS) and hard X-ray photoelectron spectroscopy (HAXPES). The former experiments were performed at the WERA beamline of ANKA, Karlsruhe, the latter at beamline P09 at PETRA III, Hamburg.

In (DOEO)<sub>4</sub>[HgBr<sub>4</sub>]·TCE we have found evidence of an antiferromagnetic phase that exists below 40 K. We characterize occupied and unoccupied electronic states in the crystals. Sulfur 2s and chlorine 2p HAXPES core-level spectra have been taken at different temperatures. They provide evidence of an electron density redistribution in DOEO layers upon cooling and correlations between phase transitions and electronic states in the crystals. Furthermore, the sulfur 2p and oxygen 1s edges have been investigated by NEXAFS, revealing fingerprints of charge carriers redistribution and localization at T<50 K. Based on temperature dependences of magnetic susceptibility, transport properties<sup>[1]</sup>, an electron spin resonance study<sup>[2]</sup> and electron density distributions we propose a mechanism of localization with appearance of antiferromagnetic islands in (DOEO)<sub>4</sub>[HgBr<sub>4</sub>]·TCE.

In TTF-TCNQ we have performed a temperature-dependent NEXAFS investigation. Although several NEXAFS studies were done on the same compound before<sup>[3,4]</sup>, we have performed the experiment at different temperatures. Our study shows an evidence of a Peierls transition on the TCNQ stacks. Furthermore, the data provide the first experimental evidence of a modification of intra-molecular orbitals due to a charge density wave (CDW) instability in a molecular conductor. In addition, we clearly resolve the experimental data, consisting of all theoretically predicted peaks, including the “missing” transition  $\sigma^*(\pi(\text{ag}, \text{b3u}))$  in the cyano groups of TCNQ, and therefore we can discuss the real electronic structure and its evolution with variable temperature.

In the last part we present NEXAFS results for molecular beam deposited thin films of triangulene and its trimethoxy derivative donors<sup>[5]</sup> in complexes with the strong F4-TCNQ acceptor in comparison with density functional theory (DFT) calculations. We have found that there is a filling of  $a_u, b_{1u}$  ( $\pi^*$ -ring) and  $b_{2g}$  ( $\pi^*$  ring) orbitals of nitrogen visible in the K-edge NEXAFS spectra during formation of the charge transfer complexes in both cases.

The experiments were funded by Transregio SFB TR49 and BMBF(project 05K13UM4). A.C. thanks the Graduate School of Excellence *Materials Science in Mainz* for financial support.

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# Spin-Polarization and Spin-Orbit Coupling in Au-Induced Atom Chains on High-Index Silicon Surfaces

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Atoms can form chain-like architectures by self-assembly on various semiconductor surfaces. Such may offer physical realizations of various one-dimensional (1D) electronic ground states like Peierls instabilities or Tomonaga-Luttinger liquids. Here we report on Au-stabilized nanowires on a high-index silicon substrate, namely Si(553). The two chain types present in that system, one built by Au and one by Si atoms, develop two- and threefold periodicities at low temperatures, which were previously assigned as Peierls instabilities. However, our results from scanning tunneling microscopy and spectroscopy are in astounding agreement with the Si(553)-Au ground state predicted by density-functional theory, where every third Si atom is spin polarized [1]. Moreover, the structural model [2] suggests strong spin-orbit coupling for the Au chains. Using spin- and angle-resolved photoemission we find direct evidence for such a spin-splitting in both Au-induced parabolic bands. In addition, we tuned the physical properties of the system by varying the high-index substrate using Si(775). This varies not only the interwire spacing, but also gives rise to new structural features affect the spin pattern. These finding render this family of nanowires an intriguing 1D material with spin ordering in both real and reciprocal space.

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# Surface / interface interaction in LaAlO<sub>3</sub>/SrTiO<sub>3</sub> heterostructures: an *in situ* transport and photoemission study

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Oxide heterostructures display many interesting phenomena, one example being the formation of a two-dimensional electron system (2DES) at the LaAlO<sub>3</sub>/SrTiO<sub>3</sub> (LAO/STO) interface beyond a critical thickness of 4 monolayers (ML) of the polar LAO [1, 2]. An explanation for this behavior is the so-called electronic reconstruction. In this context it has recently been shown that polar adsorbates can enhance the conductivity of the 2DES [3]. Besides their electrostatic influence it was discussed that surface defects/adsorbates can also act as a charge reservoir [4]. To examine the impact of surface adsorbates on the 2DES we performed *in situ* conductivity measurements and *in situ* photoelectron spectroscopy (PES) on 6ML thick LAO/STO heterostructures exposed to a defined amount of water vapor. PES experiments indicate that water adsorbates induce additional charge carriers at titanium sites which are located at the interface. We correlate these spectroscopic findings with *in situ* conductivity measurements.

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## O K-edge RIXS energy dependence of low-energy excitations in underdoped $\text{La}(2-x)\text{Sr}_x\text{CuO}_4$

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The insulator to superconductor phase boundary is a poorly understood region of the phase diagram of the cuprates. A better understanding of the electronic structure of these complex materials in this crucial region would probably represent a major step towards a theory of high temperature superconductivity. In particular, it has been proposed that persistent magnetic fluctuations could provide the pairing “glue” [1]. In this study, we have used Resonant Inelastic x-ray Scattering (RIXS), a novel probe of electronic and magnetic excitations in solids. We have investigated the low-energy excitations at O K-edge in the paradigmatic cuprate material  $\text{La}(2-x)\text{Sr}_x\text{CuO}_4$  (LSCO), as a function of doping ranging from an insulator to a bad metal (superconductor). We identify the signatures of bimagnon excitations, which persist in the underdoped superconductor. Remarkably, we have been able to resolve for the first time a double peak structure at  $\sim 2$  eV, for which previous theoretical calculations suggest a Zhang-Rice singlet nature [2-3].

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## Valence Band Electronic Structure and Band Alignment in LaAlO<sub>3</sub>/SrTiO<sub>3</sub>(111) Heterointerfaces

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Rich electronic behavior has been found to emerge at interfaces of perovskite oxides [1] since the discovery of a confined electron system between the (001) oriented wide-gap band insulators LAO and STO by Ohtomo and Hwang [2]. In (111) orientation, both STO and LAO are polar, but with a polar discontinuity of the same size as in the (001) case, meaning that in an ideal electronic reconstruction scenario also half an electron would have to be transferred to the interface in order to heal the polarization catastrophe. LAO/STO (111) samples indeed also exhibit a critical thickness for conductivity (6 bilayers corresponding to a thickness of about 14 Å) with similar mobilities and carrier concentrations as for the (001) oriented heterostructures [3]. A distinct feature of the (111) interface is its peculiar real space topology. Each bilayer represents a buckled honeycomb lattice similar to the case of graphene which is known theoretically to host various topologically non-trivial states. Bilayer STO in proximity to the interface thus can be regarded as a three-orbital (due to the three Ti 3d t<sub>2g</sub> orbitals) generalization of graphene with enhanced electron correlations making it a promising candidate for the realization of strongly correlated topological phases. Density functional theory calculations predict a wealth of interesting phases induced by symmetry breaking and electron correlations, including such with charge order, spin and orbital polarization, or topological phases with protected surface states [4].

We have depth-profiled the interface electron system by XPS of the Ti 2p core levels. Combining resonant SX-PES and HAXPES measurements has enabled us to directly probe the electronic states contributing to the 2DES and so called in-gap states at higher binding energies (~1.3 eV) as well as the Ti2p core levels and the band alignment at the same time. By dosing oxygen or by inducing oxygen vacancies with synchrotron light irradiation we can even engineer the emergence of the valence band states and the band alignment. We have furthermore mapped the momentum-resolved electronic structure of the interface Ti 3d states.

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## Students oral contributions

## Quenched Magnon dispersion by oxygen sub-lattice reconstruction in SrCuO<sub>2</sub> thin films

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Multi-layered thin films of cuprates allow studying how the crystal field and the dispersion of magnetic excitations can be sensitively modified.[1][2] In (SrCuO<sub>2</sub>)<sub>n</sub>/(SrTiO<sub>2</sub>)<sub>2</sub> superlattices, in particular, a structural transformation from a bulk planar to a pyramidal local environment has recently been observed that is driving an orbital reconstruction for  $n < 5$ . [3] Here we present results regarding the influence of this orbital reconstruction on the magnetic dispersion using resonant inelastic x-ray scattering at the Cu L<sub>3</sub> edge. A clear quenching of the magnon dispersion for SrCuO<sub>2</sub> layer thicknesses of 3 unit cells is observed.

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## Electron pair emission detected by time-of-flight spectrometers: new perspectives

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We present results for electron coincidence spectroscopy obtained by using two time-of-flight (ToF) spectrometers. Electron-pair emission from a Cu(111) surface detected in coincidence and excited by electron impact allows to resolve the dispersion of the Shockley surface state in the momentum distribution. By combining the two ToF spectrometers with a high-order harmonic generation light source opens up new perspectives to enable  $(\gamma,2e)$  spectroscopy in the laboratory that required synchrotron radiation in the past [1]. Utilizing this setup we report results for  $(\gamma,2e)$  on NiO(001) on Ag(001) excited with light at 30 eV photon energy.

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## HHG-based double photoemission spectroscopy from solids

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Light sources based on high-order harmonic generation (HHG) have a great potential because of their wide photon energy range together with the possibility for ultrafast time-resolved spectroscopy. But for advanced photoemission spectroscopy and microscopy there are limitations due to a low repetition rate, typically in kHz range, and a complicated optical setup.

In our work we combine a home-built HHG light source with photon energies tunable between 16 and 40 eV at MHz repetition rate and time-of-flight spectroscopy (ToF) [1]. Combined with two ToF spectrometers we perform double photoemission (DPE) experiments in the laboratory [2]. In DPE spectroscopy a pair of photoelectrons is excited by one single photon and detected simultaneously.

Here we present the first HHG-based DPE spectroscopy on Ag and NiO to investigate electron correlation in solids. Whereas for Ag(100) a DPE count rate of about 1 count/s is observed, the DPE count rate for strongly correlated NiO is about a factor of 4 higher at comparable single photoemission count rate. This experimental observation is in qualitative agreement with theoretical predictions, where the DPE intensity is related to the strength of electron correlation [3].

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## Tetragonal CuO: a two dimensional cuprate with novel intralayer coupling

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The cupric oxide CuO exhibits an insulating ground state with a correlation-induced charge-transfer gap and antiferromagnetism. In principle, CuO is the most straightforward parent compound of the doped cuprates, where corner sharing CuO<sub>4</sub> plaquettes host the formation and propagation of the Zhang-Rice singlet (ZRS) quasiparticle.

Bulk CuO crystallizes in a low-symmetry monoclinic form, in contrast to the rocksalt structure typical of late 3d transition metal monoxides. Recently, CuO was synthesized by epitaxial growth on SrTiO<sub>3</sub> substrates in a higher symmetry tetragonal structure much closer to the one observed in most cuprates (Siemons et al. PRB 79, 2009). At beamline 7 of the Advanced Light Source, we have grown tetragonal CuO thin films by pulsed laser deposition and revealed the dispersion of the first ionization state, a ZRS, by means of in situ angle-resolved photoemission (ARPES). We demonstrate that the ZRS preferentially propagates on two weakly coupled corner sharing sublattices in this edge sharing coordination. We will further discuss some possible implications for the magnetic ordering transition in the insulating system and for superconductivity in the doped compounds.

## The electronic structure of IrO<sub>2</sub> and Bi<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub> studied by high-resolution HAXPES and DFT

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Iridium oxide, IrO<sub>2</sub> is a conductive transition metal oxide of significant practical and theoretical interest. On the one hand, it is known to be one of the best catalysts for the oxygen evolution reaction, and as such it finds extensive use in novel water-splitting arrangements.<sup>1</sup> On the other hand, the recent spur of research activity concerned with ternary iridium-containing oxides, iridates, has also inspired a revival of interest in the fundamental properties of IrO<sub>2</sub>. For example, Clancy et al and Hirata et al have used X-ray Absorption Spectroscopy (XAS) and Anisotropic Tensor of Susceptibility (ATS) scattering respectively to find a surprisingly large degree of spin-orbit coupling for the Ir 5d valence electrons in this material.<sup>2,3</sup> In order to further our understanding of IrO<sub>2</sub>, a detailed analysis of the valence band electronic structure, and in particular the states close to the Fermi level that are responsible for the conduction properties of this material is required.

In the present study, we used high-resolution Hard X-ray Photoelectron Spectroscopy (HAXPES) in normal emission mode to obtain bulk-sensitive information about the electronic structure of IrO<sub>2</sub>. High resolution (ca 0.26eV in our measurements) is particularly desirable in the study of the valence band of IrO<sub>2</sub> due to the highly modulated density of states near the Fermi level. Additionally, electronic structure calculations were performed within the density functional theory (DFT) framework, and excellent agreement between theory and experiment was observed, as shown in the figure above.

The results of the calculations will be analyzed further in terms of the atomic orbital nature of the states in the valence band, with particular attention to the Ir 5d orbitals of "t<sub>2g</sub>"-like character that contribute most of the density of states in the vicinity of the Fermi level. Additionally, I will discuss the fitting of the iridium core level HAXPES (and XPS) spectra, as it is of significant importance to the investigation of the behaviour of IrO<sub>2</sub> in electro-chemical setups.<sup>4,5</sup> Finally, I will present recent Al K-alpha XPS and HAXPES data of another metallic iridium oxide, Bi<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub>, which is unusual amongst the iridates in that the valence orbitals of the third element, in this case Bi, are

strongly hybridized with the Ir and O based orbitals.

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## Interstellar dust studied through X-ray spectroscopy

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In this PhD project I study the dense regions of our Galaxy, using X-ray binaries (a class of binary stars that are bright in the X-rays) as background sources to probe the intervening interstellar dust. Interstellar dust plays an important role in the life cycle of stars and is present on all scales in the universe. Studying the X-ray absorption fine structures (XAFS) of the absorption edges in the spectrum enables us to determine the structure and composition of the interstellar dust. The features in the absorption edge caused by the XAFS give a fingerprint for the type of dust. In order to determine what type of dust best fits the observed spectra, we compare these spectra with laboratory data of different silicates that resemble the possible composition of the dust. We focus in particular on the features caused by the silicon and magnesium absorption. We measured magnesium and silicon absorption edges for a set of different silicates in both crystalline and amorphous form at the Soleil synchrotron facility in Paris. These absorption edges were implemented in a fitting program in order to model the interstellar dust absorption and scattering. As a test case we applied our models to a high quality spectrum of a bright background X-ray source located in the vicinity of the Galactic Center.



## Fermi states of bulk decagonal AlNiCo quasicrystal

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Quasicrystals (QCs) are intermetallic alloys which have excellent long-range order but no translational symmetry. Despite years of research, the exact mechanism of stabilization of the QC structure is still under debate. Clarification of this fundamental issue requires  $\mathbf{k}$ -resolved spectroscopic information about the states in the vicinity of  $EF$  which can be achieved by ARPES. Potential surface segregation and 3D character of most of the QC materials demand the use of soft-X-ray ARPES (SX-ARPES) with its large probing depth and improved definition of 3D momentum. Here we report first results of electronic structure investigation of decagonal Al-Ni-Co quasicrystal by means of SX-ARPES.

Fermi surface (FS) contours and valence band (VB) dispersion near Fermi level of 10-fold Al-Ni-Co were measured at different photon energies  $h\nu$  by means of Soft-X-Ray ARPES. Clear linear dichroism observed in valence band confirmed that the Fermi states are formed by symmetric dispersive Al  $3sp$  states hybridized with Co and Ni  $d$ -states. The observed FS contours were quite sharp, thus unveiling the delocalized character and sharp  $\mathbf{k}$ -definition of the valence states. Pseudogap existence near  $EF$  along the main high-symmetry valence band cuts at  $\Gamma$ - and Z-points was investigated and the stabilization mechanism is discussed.

# Temperature-dependent surface band gap of Dirac fermions observed at the (111) surface of the crystalline topological insulator Pb-Sn-Se

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Using angle-resolved photoemission, we studied (111)-oriented epitaxial films of Pb-Sn-Se grown by molecular beam epitaxy. The topological-to-trivial-insulator phase transition [1] is monitored probing the bulk valence band as a function of Sn concentration and temperature between 30 K and room temperature. In the topological phase, the topological surface state opens a band gap indicating a mass acquisition that is not caused by broken time reversal symmetry. We discuss this phenomenon in comparison to conventional topological insulators [2] protected by time-reversal symmetry.

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# Photoemission and Loss Spectra of CuO from First-Principles Many-Body Calculations

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Even though the strongly correlated transition-metal oxide CuO has many fields of application (potential absorber material in photovoltaic devices, pigment in glass and ceramics, building block of cuprate superconductors,...), surprisingly little is known about its electronic excitations from a theoretical point of view. The band gap and all electronic excitations in its vicinity are governed by the intricate interplay between itinerant O 2p and localized Cu 3d electrons. Complex many-body effects, that are still not well understood nowadays, determine the screening of the electron-electron interaction.

We use the GW method of many-body Green's function theory to calculate electron and hole quasiparticle excitations in CuO and compare them to direct and inverse photoemission spectra. Matrix-element and lifetime broadening effects are taken into account. In particular, the band-gap issue is addressed. Furthermore, time-dependent density-functional theory (TDDFT) is employed to calculate the frequency- and wave-vector-dependent loss function of CuO. The occurring d-d and plasmon excitations are discussed. Comparison with recent experimental data from non-resonant inelastic x-ray scattering (NIXS) allows us to assess the quality of the calculated screened Coulomb interaction  $W$  which is a key ingredient in various many-body approaches, for instance, GW and Bethe-Salpeter calculations.

# Monochromatization of femtosecond XUV light pulses with the use of reflection zone plates for time resolved photoelectron spectroscopy.

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We present a newly built laser-based tabletop setup for time resolved photoelectron spectroscopy [1]. The system consists of an optical parametric amplifier giving femtosecond laser radiation in the ultraviolet to infrared regime to excite the sample, whereas femtosecond extreme ultraviolet (XUV) light generated as high harmonic (HHG) from a titanium sapphire laser is used as the probe. The key feature of this setup is the monochromator inducing only low temporal broadening of the XUV pulses whilst maintaining a high transmission. This monochromator employs off-center reflection zone plates as diffracting and focusing element. It shows to be superior to gratings when selection of a desired harmonic is carried out with the use of a single optical element. The function of the monochromator as well as the spatial, spectral, and temporal characteristics of the monochromized XUV beam will be presented.

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## Angle-resolved photoemission spectroscopy of the isovalent-substituted Fe-based superconductor $\text{SrFe}_2(\text{As}_{0.65}\text{P}_{0.35})_2$

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Isovalent-substituted iron pnictide superconductor  $\text{SrFe}_2(\text{As}_{1-x}\text{P}_x)_2$  and the similar well-known system  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$  share the almost same pnictogen heights and are both considered to have superconducting gap nodes from penetration depth measurements, whereas the  $c$ -axis length is significantly shorter in  $\text{SrFe}_2(\text{As}_{1-x}\text{P}_x)_2$  than in  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$  reflecting the smaller atomic radius of Sr atoms.  $\text{SrFe}_2(\text{As}_{1-x}\text{P}_x)_2$  ( $x = 0.35$ ,  $T_c = 33$  K) has a slightly higher optimum critical temperature than  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$  ( $x = 0.30$ ,  $T_c = 30$  K), and its parent compound  $\text{SrFe}_2\text{As}_2$  has a much higher Néel temperature ( $T_N = 197$  K) than  $\text{BaFe}_2\text{As}_2$  ( $T_N = 142$  K) [1]. In order to investigate how the change in the  $c$ -axis length affects the electronic properties and the superconducting gap structures, we have performed an angle-resolved photoemission spectroscopy measurement on  $\text{SrFe}_2(\text{As}_{1-x}\text{P}_x)_2$  [2]. Measurements with different photon energies have revealed that the outermost hole Fermi surface (FS) is more strongly warped along the  $k_z$  direction than the corresponding one in  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ , and that the innermost one becomes a 3D ellipsoidal pocket. Comparison of the ARPES data with first-principles band-structure calculation revealed that the quasi-particle mass renormalization factors are significantly higher than those of  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ . While the three hole FSs show orbital-dependent superconducting gaps, the electron FSs have almost isotropic and  $k_z$ -independent superconducting gaps.

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## Calculation of SPLEED patterns, target current and ARPES for various surface systems

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The combination of experiment and theory plays a important role especially for scientific fields like material science. One boundary for the conclusive comparison of theory and experiment is, of course, the spectroscopic investigation of materials including all its different methods. Using the fully relativistic KKR-method [1] in the framework of DFT (Density Functional Theory) we are able to calculate the electronic structure and on top different spectroscopic properties of various materials. We show results for the calculation of SPLEED (Spin-Polarized Low-Energy Electron Diffraction) patterns for the system Fe(001)-p(1x1)-O. Due to the low energies of the incident electrons considered we use a complete relaxed surface and interface structure [2]. Furthermore, we investigate the inclusion of many body effects within the framework of DMFT (Dynamical Mean Field Theory) when calculating SPLEED-spectra. Additionally we included the reduced projection of the polarization of the incident electron due to a change of the polar angle. It is shown that this effect has a significant impact on the theoretical results. Beside the scattered intensities of the spin-polarized electrons another quantity useful for the characterization of a crystal surface is the target current, i.e. the absorptive part of the incident electron intensity [3]. We show results for calculations of the target current for different electron energies and polar angles. Finally it is shown that the KKR-method provides the basis for a effective calculation of ARPES (Angle-Resolved Photoemission Spectroscopy) [4]. For all of our calculations a comparison between theory and experiment is made [4, 5]

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# Ultrafast study of Cr:W(110) Thin Films

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Chromium is a textbook example of an itinerant antiferromagnet, and its rich phase diagram which includes both spin and charge density waves has been widely studied [1]. Of particular interest is the complex interplay which exists between the density wave phases; the mechanism of which is still under debate [2].

Time and angle resolved photoemission spectroscopy (trARPES) allows access to both the electronic band structure of solids and the lifetimes and many body interactions of the constituent particles and quasi-particles [3]; complementary to high resolution ARPES. Until now this technique has not been applied to chromium thin films.

We employ trARPES to study Cr thin films grown on a W(110) substrate. The ultrafast dynamics reveal both a shift of the chemical potential and a rigid shift of the band structure on a timescale of a few hundred femtoseconds. We interpret the former as a direct consequence of particle conservation through the spin density wave transition and the latter as a result of the transient disequilibrium between the chemical potentials of the Cr film and the analyser.

We model the experimental band structure, including a BCS type description of the spin density wave phase transition, in conjunction with a two-temperature-model to better understand how the temperatures of different sub-systems impact on the ultrafast dynamics of chromium. Such dynamics afford insights into the hot electron transport in these thin films and furthermore hint at the nature of spin density wave transition.

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# Bulk electronic structure of quasicrystals studied by HAXPES

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We have used hard x-ray photoelectron spectroscopy (HAXPES) to investigate the bulk electronic structure of quasicrystals to resolve the controversy about the existence of pseudogap in these materials. Here, we report results of our studies on icosahedral Al-Pd-Mn, Al-Cu-Fe and rare earth based Zn-Mg-Dy quasicrystal at low temperature (40K), recorded with 8 and 6 keV photon energies. The near  $E_F$  spectra of Al-Pd-Mn as well as Al-Cu-Fe are strongly suppressed in intensity at  $E_F$ , which provides strong evidence for the existence of the pseudogap in contrast to surface sensitive low energy photoemission spectra that shows a metallic Fermi edge. To quantify the depth and the width of the pseudogap, we have fitted the near  $E_F$  spectra by using an inverted Lorentzian function. We find that for Al-Pd-Mn, the depth of the pseudogap is 72%, whereas for Al-Cu-Fe it is 100 %. This means that the pseudogap is fully formed in case of Al-Cu-Fe [1]. On the other hand, surface sensitive low energy photoemission spectra reveals that the depth is 28% and 56% for Al-Pd-Mn and Al-Cu-Fe, respectively, indicating that the pseudogap is much shallower in the surface compared to the bulk. The evidence of fully formed pseudogap in Al-Cu-Fe demonstrate that the DOS at  $E_F$  is zero indicating that it is close to a metal-insulator phase boundary, in agreement with the specific heat and transport measurements [2]. The existence of deeper pseudogap in bulk has been supported by the theoretical calculations [3]. HAXPES valence band spectrum of Al-Pd-Mn exhibits that the Pd 4d peak is shifted by about 0.3 eV compared to the surface and this is related to a bulk versus surface effect, possibly enhanced by excess Pd at the surface. A similar effect is also observed for Al-Cu-Fe: the Cu 3d main peak at 4.6 eV is shifted by 0.6 eV towards higher binding energy. The near  $E_F$  spectrum of Zn-Mg-Dy exhibits shallower pseudogap (44%) compared to the Al based quasicrystals (Al-Pd-Mn and Al-Cu-Fe). This is also in agreement with transport measurement that show one order of magnitude larger carrier concentration in Zn-Mg-Dy compared to Al-Pd-Mn [4]. The evidence of Van hove singularity in the near  $E_F$  spectra of rare earth based quasicrystals had been demonstrated from low energy photoemission measurement. However, our HAXPES measurements do not exhibit any signature of Van hove singularity in Zn-Mg-Dy.

## References

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## PLANNING FOR STUDENTS' TALKS

Each talk is 15 minutes + 10 minutes questions/discussions

### Session 1: Friday 5 September

- 18h00 – 18h25: Stephan Borek  
*Calculation of SPLEED patterns, target current and ARPES for various surface systems*
- 18h25 – 18h50: Claudia Rödl  
*Photoemission and Loss Spectra of CuO from First-Principles Many-Body Calculations*
- 18h50 – 19h15: Simon Moser  
*Tetragonal CuO: a two dimensional cuprate with novel intralayer coupling*

### Session 2: Saturday 6 September

- 16h00 – 16h25: Andreas Trützchler  
*HHG-based double photoemission spectroscopy from solids*
- 16h25 – 16h50: Michael Huth  
*Electron pair emission detected by time-of-flight spectrometers: new perspectives*
- 16h50 – 17h15: Sascha Zeegers  
*Interstellar dust studied through X-ray spectroscopy*

### Session 3: Saturday 6 September

- 17h45 – 18h10: Hakuto Suzuki  
*Angle-resolved photoemission spectroscopy of the isovalent-substituted Fe-based superconductor  $SrFe_2(As_{0.65}P_{0.35})_2$*
- 18h10 – 18h35: Victor Rogalev  
*Fermi states of bulk decagonal ALNiCo quasicrystal*
- 18h35 – 19h00: Jayita Nayak  
*Bulk electronic structure of quasicrystals studied by HAXPES*

### Session 4: Friday 12 September

- 8h45 – 9h10: Marcus Dantz  
*Quenched Magnon dispersion by oxygen sub-lattice reconstruction in SrCuO<sub>2</sub> thin films*
- 9h10 – 9h35: Jan Metje  
*Monochromatization of femtosecond XUV light pulses with the use of reflection zone plates for time resolved photoelectron spectroscopy*
- 9h35 – 10h00: Chris Nicholson  
*Ultrafast study of Cr:W(110) Thin Films*

### Session 5: Friday 12 September

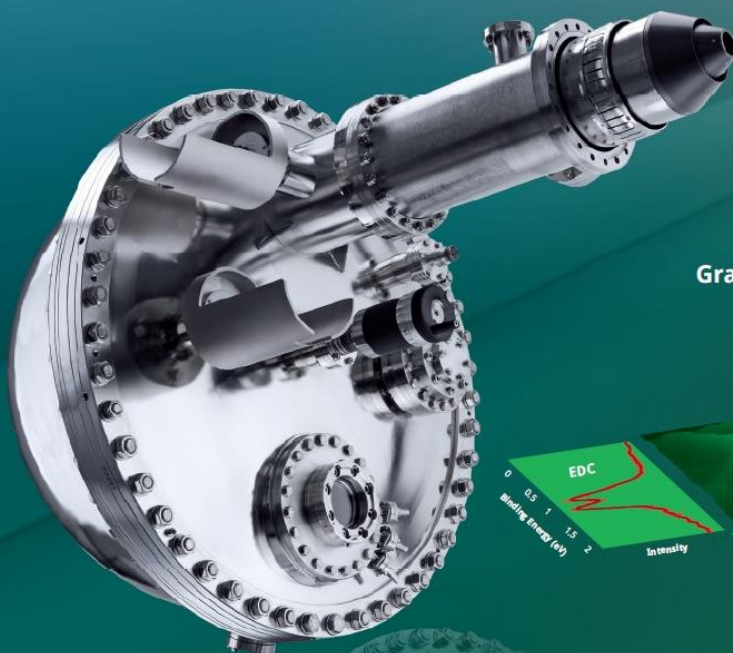
- 10h15 – 10h40: Partha Sarathi Mandal  
*Temperature-dependent surface band gap of Dirac fermions observed at the (111) surface of the crystalline topological insulator Pb-Sn-Se*
- 10h40 – 11h05: Juhan Matthias Kahk  
*The electronic structure of IrO<sub>2</sub> and Bi<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub> studied by high-resolution HAXPES and DFT*

# PHOIBOS 225

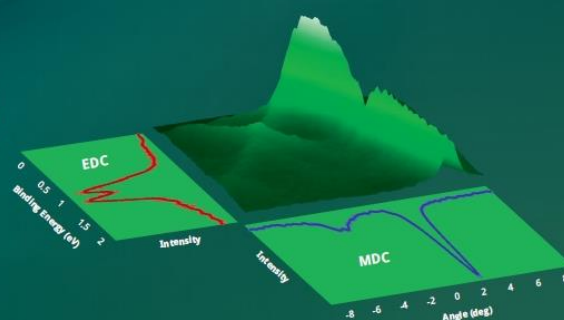
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## KEY FEATURES

- Ultra High Energy Resolution in UPS (<1 meV)
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