CoRPES15

International workshop on strong correlations and angle-resolved photoemission spectroscopy

5th to 10th of July 2015

Couvent des Cordeliers (Paris, France)

TOPICS

Spectroscopic investigations of quantum materials

Many-body theory of correlated electrons in solids

The photoemission process

Advances in ARPES resolution: time, space and spin

Relations to other photon-based techniques

Scientific Committee

Philippe Aebi - Université de Fribourg, Switzerland
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Jean-Marc Lucacchioni
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Amina Taleb-Ibrahimi
Stéphanie Yao

Invited speakers

Uwe Bovensiepen
Yulin Chen
Andrea Damascelli
Hugo Dil
Hong Ding
Hubert Ebert
Donglai Feng
Martin Ganahl
Antoine Georges
Giacomo Ghiringhelli
Kristjan Haule
Philip Hofmann
Masatoshi Imada
Lex Kemper
Bum Joon Kim
Takeshi Kondo
Eugene Krasovskii
Jan Kunes
Alessandra Lanzara
Luca Perfetti
Georges Sawatzky
Anna Tamai
Inna Vishik
Philipp Werner

www.synchrotron-soleil.fr/Workshops/2015/CORPES2015

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SOLEIL SYNCHROTRON

International Workshop on Strong Correlations and Angle-resolved Photoemission Spectroscopy
CORPES15

Couvent des Cordeliers, Paris, France
05th-10th of July 2015

Conference organization:

Sponsors:

Poster Awards:

International Workshop on Strong Correlations and Angle-resolved Photoemission Spectroscopy
CORPES15

Couvent des Cordeliers, Paris, France
05th-10th of July 2015

Summary

CORPES15

International workshop on strong correlations and angle-resolved photoemission spectroscopy

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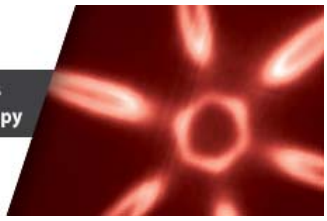
Couvent des Cordeliers (Paris, France)



Welcome

CORPES is an interdisciplinary workshop whose scope is situated at the crossroads between photoemission spectroscopy and many-body theory. The main goal is to advance our understanding of strongly correlated materials using angle-resolved photoemission as a unique tool to access their electronic structure and many-body theory to work out the underlying concepts and mechanisms. Not only the characteristics of correlated quantum matter but also those of novel materials such as topological insulators, and the photoemission process itself will be addressed. The discussion of prospects and challenges brought up by new light sources, novel experimental techniques and innovative theoretical ideas are central to the CORPES forum.

CORPES-15 is organized by the SOLEIL Synchrotron in the center of Paris on July 5-10th, 2015. It follows the scope and motivation of the previous workshops CORPES-05 and CORPES-07 held in Dresden, CORPES-09 in Zurich, CORPES-11 in Berkeley and CORPES-13 in Hamburg.

The program is a balanced fusion of currently well-established and newly emerging topics. It is intended to bring together experts and newcomers in the field, to learn from one another, and to foster collaborations. We have preserved the workshop spirit, i.e., a linear schedule with no parallel sessions and ample time for discussion after each presentation as well as between sessions. Applicants to the workshop have been selected to give either oral or poster presentations, with the latter being given significant weight to the program including short oral poster « flash sessions ».

Bienvenue

CORPES est un colloque interdisciplinaire qui se situe à l'intersection entre la spectroscopie de photoémission et les théories à N corps. Son but principal est d'avancer notre compréhension des systèmes fortement corrélés en utilisant la photoémission résolue en angle comme technique permettant d'accéder à leur structure électronique et les théories à N corps comme outils pour modéliser les concepts et mécanismes sous-jacents. Nous ne nous intéresserons pas seulement aux propriétés de la matière corrélés mais aussi à celles de nouveaux systèmes comme les isolants topologiques et au processus de photoémission lui-même. Nous discuterons également les perspectives et défis apportés par les nouvelles sources de lumière, des nouvelles techniques expérimentales ou des idées théoriques innovantes, qui sont tous des aspects essentiels du colloque CORPES.

CORPES-15 est organisé par le synchrotron SOLEIL au centre de Paris du 5 au 10 juillet 2015. Il continue la tradition établie par les précédentes éditions de CORPES-05 et CORPES-07 à Dresde, CORPES-09 à Zurich, CORPES-11 à Berkeley et CORPES-13 à Hambourg.

Le programme maintient un équilibre entre des sujets bien établis et des sujets émergents. Son intention est de rassembler des experts et des nouveaux venus dans le domaine, d'apprendre les uns des autres et de susciter des collaborations. Il préserve l'esprit d'un colloque, en évitant les sessions parallèles, et en laissant du temps pour les discussions après chaque présentation et entre les sessions. Les participants au colloque ont été sélectionnés pour donner soit des présentations orales, soit des posters. Un poids important est accordé dans le programme aux posters, qui seront aussi annoncés par oral dans des sessions « flashs ».

International Workshop on Strong Correlations and Angle-resolved Photoemission Spectroscopy
CORPES15
Couvent des Cordeliers, Paris, France
05th-10th of July 2015

COMMITTEES

Conference chair

Véronique BROUET	LPS Orsay, CNRS-Université Paris Sud, France

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International Workshop on Strong Correlations and Angle-resolved Photoemission Spectroscopy
CORPES15

Couvent des Cordeliers, Paris, France
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Programme

Sunday, July 5th

16:30 - 19:00 Registration & Welcome cocktail

Monday, July 6th

08:00 - 09:00 Registration
09:00 - 09:20 Opening & Welcome

Chairperson: Véronique BROUET

09:20 - 09:50 Bad metals and Hund's metals: Spectroscopies and transport
Antoine Georges *- Collège de France, Paris et Ecole Polytechnique, Palaiseau, France*

09:50 - 10:20 Mechanism and manipulation of superconductivity in FeSe thin films
Donglai Feng *- Fudan university, Shanghai China*

10:20 - 10:40 Connection between high-energy spin-excitations and degree of electron correlations in $Ba(Fe_{1-x}Cox)_2As_2$ superconductors
Yaobo Huang *- Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland*

10:40 - 11:10 Coffee break

Chairperson: James FREERICKS

11:10 - 11:40 Theoretical studies of non-equilibrium spectroscopy
Alexander Kemper *- Lawrence Berkeley National Laboratory, Berkeley, USA*

11:40 - 12:00 Ultrafast gap dynamics in $Bi_2Sr_2CaCu_2O_{8+\delta}$ studied by high resolution trARPES
Stephen Parham *- University of Colorado, Boulder, USA*

12:00 - 12:20 Ultrafast surface and bulk carrier dynamics in photo-excited topological insulators
Evangelos Papalarazou - *LPS, Université Paris Sud, Orsay, France*

12:20 - 14:30 Lunch

Chairperson: Daniel DESSAU

14:30 - 15:00 Non-equilibrium momentum dependent dynamic of high temperature superconductors
Alessandra Lanzara *- University of California, Berkeley, USA*

15:00 - 15:30 Thermalization of photo-excited Mott insulators
Philipp Werner *- University of Fribourg, Fribourg, Switzerland*

15:30 - 15:50 Combining soft X-ray ARPES and STM with DFT and many-body correlations to understand the multiple aspects of the charge density wave in $TiSe_2$
Gaël Monney *- Fribourg Center for Nanomaterials*, *University of Fribourg, Fribourg, Switzerland*

15:50 - 16:10 Accessing the self-energy of a correlated material with time-resolved ARPES
Claude Monney - *University of Zurich, Zurich, Switzerland*

16:10 - 16:40 Coffee break

Chairperson: Ashish CHAINANI

16:40 - 17:10 Superconducting mechanisms of iron-based and cuprate superconductors
Masatoshi Imada - *Department of Applied Physics - University of Tokyo, Japan*

17:10 - 17:30 Superconducting instabilities, spectral functions and quasiparticle interference in iron-based superconductors
Ilya Eremin *- Institut für Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany*

17:30 - 17:50 High-energy electronic interaction in iron-based superconductors
Daniil Evtushinsky *- Institute for Solid State Research, IFW Dresden, Dresden, Germany*

17:50 - 18:10 Tuning electronic correlations in transition metal pnictides: Chemistry beyond the Valence count
Elia Razzoli - *Swiss Light Source, Paul Scherrer Institute, Villigen*, *and Fribourg Center for Nanomaterials, University of Fribourg, Switzerland*

Tuesday, July 7th

Chairperson: Silke BIERMANN

09:00 - 09:20 Charge order in cuprates: From hole to electron doping
Andrea Damascelli *- Department of Physics and Astronomy, University of British Columbia,Vancouver, Canada.*

09:20 - 09:50 Resonant X-ray scattering of cuprates: Where inelastic and elastic meet
Giacomo Ghiringhelli *- CNR/SPIN and Dipartimento di Fisica, Politecnico di Milano, Milano, Italy*

09:50 - 10:20 What does resonant inelastic X-ray scattering at the Cu L edge really measure?
Krzysztof Wohfeld *-SLAC National Laboratory and Stanford University, Menlo Park, USA and Institute of Theoretical Physics, University of Warsaw, Poland*

10:20 - 10:40 Charge excitations in resonant inelastic X-ray scattering: Detecting enhanced small-momentum charge fluctuation of electron-doped cuprates
Takami Tohyama - *Department of Applied Physics, Tokyo University of Science, Japan*

10:40 - 11:10 Coffee break

Chairperson: Luc PATTHEY

11:10 - 11:40 Spin textures of polar and ferroelectric materials
Hugo Dil *- Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

11:40 - 12:00 Metal-insulator transitions and magnetism in oxide interfaces
Frank Lecherman *- Institute for Theoretical Physics, University of Hamburg, Hamburg, Germany*

12:00 - 12:20 Two dimensional electron gases at the (001) and (101) surfaces of TiO_2-anatase: Role of oxygen vacancies and UV-irradiation
Patrick Le Fèvre *- Synchrotron SOLEIL, Saint-Aubin, France*

12:20 - 14:30 Lunch

Chairperson: Philipp AEBI

14:30 - 15:00 Fermi pockets and pseudogap in ligthly doped strontium iridates
Anna Tamai *- Department of Quantum Matter Physics, University of Geneva, Geneva, Switzerland*

15:00 - 15:30 Fermi arcs and their evolution in electron doped Sr_2IrO_4
Bum joon Kim *- Max Planck Institute for Solid State Research, Stuttgart, Germany*

15:30 - 15:50 Uncovering spin-polarised bulk electronic states in inversion-symmetric WSe_2
Jonathon Riley *- University of St Andrews, St Andrews, Fife, UK*

15:50 - 16:10 Nonempirical calculation of transition temperature for fulleride superconductivity
Yusuke Nomura *- Department of Applied Physics, The University of Tokyo, Tokyo, Japan*

16:10 - 16:40 Coffee break

Chairperson: Konrad MATHO

16:40 - 17:10 Point node gap persisting beyond Tc in Bi2212
Takeshi Kondo *- Institute for Solid State Physics, The University of Tokyo, Tokyo, Japan*

17:10 - 17:50 Flash Poster I

17:50 - 20:40 Poster Session I and *Dinner Buffet*

Wednesday, July 8th

Chairperson: Michael POTTHOFF

09:00 - 09:30 Hunds metallicity as the origin of anomalous state of matter in iron pnictides and chalchogenides
Kristjan Haule *- Serin Physics Lab, Rutgers University, Piscataway, USA*

09:30 - 10:00 Matrix product states based impurity solvers for dynamical mean field theory
Martin Ganahl - *Perimeter Institute for Theoretical Physics, Waterloo*, *Canada*

10:00 - 10:20 ARPES study of the electronic structure evolution in superconducting FeSe
Timur Kim *- Diamond Light Source, Didcot, UK*

10:20 - 10:40 Detailed study of the dramatic reconstruction of the electronic structure of FeSe in the orthorhombic phase
Joseph Mansart - *LPS, Université Paris-Sud, Orsay , France*

10:40 - 11:10 Coffee break

Chairperson: Takami TOHYAMA

11:10 - 11:40 Visualizing electronic structures of topological quantum materials
Yulin Chen *- Physics Department, University of Oxford, Oxford, UK*

11:40 - 12:00 Theory of Floquet band formation and local pseudospin textures in pump-probe photoemission of graphene
James Freericks *- Department of Physics**,** Georgetown University, Washington, USA*

12:00 - 12:20 Spin dynamics of hot carriers in the topological insulator Bi_2Se_3
Cephise Cacho - *Central Laser Facility, STFC Rutherford Appleton Laboratory, UK*

12:20 - 18:10 Lunch & Visit to SOLEIL beamlines

Thursday, July 9th

Chairperson: Serguei MOLODTSOV

09:00 - 09:30 Dynamics of electronic states in correlated materials and high temperature superconductors
Luca Perfetti - *LSI, Ecole Polytechnique, Palaiseau, France*

09:30 - 10:00 Electronic and bosonic excitations in high temperature superconductors analyzed by time-resolved ARPES
Uwe Bovensiepen - *Univ. Duisburg-Essen, Faculty for Physics, Duisburg, Germany*

10:00 - 10:20 Probing the atomic scale magnetic structure via spin-flip, orbital-flip and chiral excitations in resonant photoemission
Fabiana Da Pieve *- LSI, Ecole Polytechnique, Palaiseau, France*

10:20 - 10:40 Soft-X-ray ARPES investigation of chromium dioxide: More insight into the electronic correlation
Federico Bisti - *Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland*

10:40 - 11:10 Coffee break

Chairperson: Amina TALEB-IBRAHIMI

11:10 - 11:40 Elastic and inelastic scattering in attosecond streaking spectroscopy of solids
Egene Krasovkii - *University of the Basque Country and Donostia International Physics Center, San Sebastian/Donostia, Spain and IKERBASQUE, Bilbao, Spain*

11:40 - 12:20 Flash poster II

12:20 - 15:10 Lunch and Poster Session II

Chairperson: Amina TALEB-IBRAHIMI

15:10 - 15:40 Explicit role of O 2p states in high oxidation state (transition metal) oxides
Georges Sawatsky *- University of British Columbia, Vancouver, Canada*

15:40 - 16:10 Low energy excitations in cuprate high temperature superconductors
Inna Vishik *- Massachusetts Institute of Technology, Cambridge, USA*

16:10 - 16:40 Coffee break

Chairperson: Maria Carmen ASENSIO

16:40 - 17:10 Excitonic condensation of strongly correlated electrons
Jan Kunes *- Institute of Physics AS CR, Praha, Czech Republic*

17:10 - 17:30 Theoretical spectroscopy for correlated materials: Rethinking the interface of electronic structure and many-body theory
Silke Biermann *- Centre de Physique Théorique, Ecole Polytechnique, Palaiseau, France*

17:30 - 17:50 Direct observation of momentum-dependent heavy fermionic electronic structure for $CeNi_2Ge_2$
Yasuhiro Nakatani *- Osaka University, Osaka, Japan*

17:50 - 18:10 Symmetry of the Fermi surface and evolution of the electronic structure across the paramagnetic-helimagnetic transition in MnSi/Si(111)
Alessandro Nicolaou - *Synchrotron SOLEIL, Saint-Aubin, France*

20: 30 Meeting point «PILIER NORD» at the Eiffel Tower

21:00 - 23:00 Conference Dinner at the Eiffel Tower

Friday, July 10th

Chairperson: Antonio TEJEDA

09:00 - 09:30 Electronic structure and electron dynamics in two-dimensional materials
Philip Hoffman *- Department of Physics and Astronomy, Arhus University, Arhus, Denmark*

09:30 - 10:00 Discovery of Weyl semimetal TaAs
Hong Ding *- Institute of Physics, Chinese Academy of Sciences, Beijing, China*

10:00 - 10:20 Topological phases at oxide interfaces: Material-specific insight from DFT+DMFT
Oleg Janson *- Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria*

10:20 - 10:40 Non-topological 2DEG at the surface of YbB_6 and divalent hexaborides
Jonathan Denlinger - *Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, USA*

10:40 - 11:10 Coffee break

Chairperson: Jean-Pascal RUEFF

11:10 - 11:40 Spin polarization of surface states probed by ARPES
Hubert Ebert - *LMU, University of Munich, Munich, Germany*

11:40 - 12:00 Complete determination of molecular orbitals by measurement of phase symmetry and electron density
Achim Schöll - *Experimentelle Physik 7, University of Würzburg, Würzburg, Germany*

12:00 - 12:20 First nanoARPES user facility available at SOLEIL: An effective band structure probe in nanoscience
Chaoyu Chen *- Synchrotron SOLEIL, Saint-Aubin, France*

12:20 - 13:00 Poster Awards
CORPES 17
Closing

ABSTRACTS

Monday, July 6th, 2015

CORPES15

Monday, July 6th

Chairpersons: V. Brouet, J. Freericks, D. Dessau, A. Chainani

IT-EX-01 Bad metals and Hund's metals: Spectroscopies and transport
A. Georges

IT-EX-02 Mechanism and manipulation of superconductivity in FeSe thin films
D. Feng

OC-EX-01 Connection between high-energy spin-excitations and degree of electron correlations in $Ba(Fe_{1-x}Cox)_2As_2$ superconductors
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OC-EX-04 Combining soft X-ray ARPES and STM with DFT and many-body correlations to understand the multiple aspects of the charge density wave in $TiSe_2$
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IT-TH-06 Superconducting mechanisms of iron-based and cuprate superconductors
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OC-EX-07 High-energy electronic interaction in iron-based superconductors
D. Evtushinsky

OC-EX-08 Tuning electronic correlations in transition metal pnictides: Chemistry beyond the Valence count
E. Razzoli

Bad Metals and Hund's Metals: Spectroscopies and Transport

A. Georges

Collège de France, Paris et Ecole Polytechnique, Palaiseau, France

Mechanism and Manipulation of Superconductivity in FeSe Thin Films

D. Feng

State key laboratory of surface physics, and Department of physics, Fudan University, Shanghai 200433, China

ABSTRACT

The record of superconducting transition temperature (Tc) has long been 56 K for the bulk iron-based high temperature superconductors (Fe-HTS's). Recently, in single layer FeSe films grown on SrTiO3 substrate, signs for a new 65 K Tc record are reported. Combining MBE, and in situ STM and ARPES, we study the ultra thin FeSe films on various substrates. We substantiate the presence of spin/orbital ordering instability in FeSe films, a key ingredient of Fe-HTS that was missed in FeSe before, which weakens with increased thickness or reduced strain. We demonstrate that the superconductivity occurs when the electrons transferred from the oxygen-vacant substrate suppress the otherwise most pronounced spin-ordering instability in single layer FeSe. The anisotropic superconducting gap, and the QPI behaviors and impurity-induced state observed by STM both strongly suggest that the pairing symmetry of the monolayer FeSe thin film is a plain s-wave without any sign change. We establish the phase diagram of FeSe vs. lattice constant that contains all the essential physics of Fe-HTS's. With first principle calculations, we show that the superexchange interactions across Fe-As-Fe is enhanced with increased lattice constant.

By fabricating FeSe/STO/KTO and FeSe/BTO/KTO hetero-structures to expand the lattice, we further tune the lattice constant of FeSe films, and increased the gap-closing temperature up to 75K. However surprisingly, Tc of 70K is observed in films with much small lattice constant as well. Moreover, we show that the high Tc cannot sustain away from the interface, and the interface has a highly nontrivial role on the electron correlations and phonon behavior. These rich behaviors pose questions on the exact role of the interface and the exact paring mechanism of such high temperature interfacial superconductors, which remain to be answered.

REFERENCES

1. S. Tan et al. Nature Materials **12**, 634 (2013).
2. H.-Y. Cao, et al. Physical Review B **89**, 014501 (2014).
3. R. Peng et al. Physical Review Letters **112**, 107001 (2014).
4. R. Peng, et al. Nature Comm. **5**, 5044 (2014).

Connection between High-energy Spin-excitations and Degree of Electron Correlations in $Ba(Fe_{1-x}Co_x)_2As_2$ Superconductors

Y. B. Huang[1, 2], J. Pelliciari[1], V. Bisogni[1,3], P. Olalde-Velasco[1], Z. P. Yin[4], K. J. Zhou[5], M. Dantz[1], G. F. Chen[2], V. N. Strokov[1], G. Kotliar[4], H. Ding[2] and T. Schmitt[1]

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[5] *Diamond Light Source, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, UK.*

ABSTRACT

Iron-based superconductors have attracted great scientific interests since their discovery. Study of the relationship between magnetism and unconventional superconductivity (SC) in this material class has been one important research focus. Spin-excitations are found to ubiquitously exist in different families of iron-pnictide superconductors [1, 2] and experimental evidence from both Inelastic Neutron Scattering and Angle-Resolved Photoemission Spectroscopy showed a close link between low-energy spin-excitations and SC [1, 3]. Our previous Resonant Inelastic X-ray Scattering (RIXS) investigation on the 122 parent compound $BaFe_2As_2$ and its optimally hole-doped superconductor $Ba_{0.6}K_{0.4}Fe_2As_2$ revealed robust high energy spin modes in both, magnetic and superconducting phases, indicating that the spin fluctuations in these materials are originating from a distinctly correlated spin state and suggesting a possible connection between magnetism and SC [4].

In order to understand the electron-hole asymmetry of the SC phase diagram in the 122 family, we probe in this study the high-energy spin-excitations in the electron-doped superconductors $BaFe_{2-x}Co_xAs_2$ with Fe-L_3 edge RIXS. Our results reveal for all doping levels well-defined spin-excitations dispersing up to 200 meV and persisting well into the superconducting phase, similar as found for the parent and the optimally hole-doped compound [4].

The energy dispersion of the high-energy spin-excitations in $BaFe_{2-x}Co_xAs_2$ is nearly independent of electron doping, displaying even slight hardening for the over-doped sample, in contrast to $Ba_{1-x}K_xFe_2As_2$ that get systematically softened with increasing of hole-doping [5]. The fact that electron-doping $BaFe_2As_2$ does not affect significantly the high-energy spin-excitations is consistent with our DMFT calculations, which show a lower degree of electron correlations for the electron-doped iron-pnictides.

Below is an example equation created with Word 97's Equation Editor. To move this equation, highlight the entire line, then use cut and paste to the new location. To use this as a template, select the entire line, then use copy and paste to place the equation in the new location.

REFERENCES

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2. R. A. Ewings, *et.al*., *Phys. Rev. B* **78** 220501(R) (2008)；S. I. Shamoto, *et.al.*, *Phys. Rev. B* **82** 172508 (2010)， T. J. Liu, *et.al*., *Nature Materials* **9** 718 (2010)
3. P. Richard, *et. al.*, *PRL* **102**, 047003 (2009)
4. K. J. Zhou, Y. B. Huang, H. Ding, T. Schmitt, *et.al., Nature Communications* **4** 1470(2013)
5. K. J. Zhou, Y. B. Huang, H. Ding, T. Schmitt, et al., unpublished.

Theoretical Studies of Non-equilibrium Spectroscopy

A. F. Kemper

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ABSTRACT

I will present some recent theoretical results regarding non-equilibrium spectroscopy. First, we study the response of a system of electrons and phonons, and what can be learned by analyzing the return to equilibrium after excitation by a laser pulse. Using a non-equilibrium Keldysh formalism, we make a connection between the observed return to equilibrium and the underlying interaction, expressed through the self-energy[1,2]. We find that the dynamics and self-energy are fluence- and time-dependent due to the modification of the electron population, which in turn modifies the interactions[3].

Second, I will present some aspects of non-equilibrium physics in BCS superconductors. We solve the Nambu-Gor'kov equations for superconductivity within the Migdal-Eliashberg approximation, obtaining a full dynamic description of non-equilibrium BCS superconductivity. The temporal behavior after a pump exhibits characteristic 2D oscillations, which we attribute to the Higgs, or amplitude mode[4]. Finally, motivated by recent experiments[5], I will illustrate how superconductivity can be enhanced or suppressed through non-linear phononics. By modifying the physical parameters, we can model the driving of a lattice distortion, leading to an enhanced Tc[6].

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2. Michael Sentef, A.F. Kemper, B. Moritz, and T.P. Devereaux, Phys. Rev. X 3, 041033 (2013)
3. A.F. Kemper, M.A. Sentef, B. Moritz, J.K. Freericks and T.P. Devereaux, Phys. Rev. B 90, 075126 (2014).
4. A. F. Kemper, M. A. Sentef, B. Moritz, J. K. Freericks, and T. P. Devereaux, arXiv:1412.2762
5. M. Först et al., Nature Physics 7, 854 (2011)
6. M. A. Sentef, A. F. Kemper, A. Georges, and C. Kollath, in preparation

Ultrafast Gap Dynamics in $Bi_2Sr_2CaCu_2O_{8+\delta}$ Studied by High Resolution trARPES

S. Parham[1], H. Li[1], J.A. Waugh[1], X.Q. Zhou[1], T. Nummy[1], J. Griffith[1], Z. Xu[2], J. Schneeloch[2], R.D. Zhong[2], G. Gu[2], D.S. Dessau[1]

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ABSTRACT

High Temperature Superconductivity is one of the prime examples of highly correlated quantum matter and its study has fueled many technological advances in the field of photoemission spectroscopy, particularly the advent of time-resolved ARPES (trARPES) [1]. Here we present a trARPES study on the gap structure of the high-T_c superconductor BSCCO-2212 using a low-energy pump (60-310 meV) to more selectively probe the electrons near the intrinsic gap scale. Previous studies have shown that the gap and superconducting quasiparticles decay on several picosecond scale [2]. We can therefore use high energy resolution pulses to study the gap in fine detail while still keeping the pulses fast enough to measure the decay lifetimes. Our findings indicate a stark contrast in the temporal dynamics of particles inside the gap-scale versus those above E_F. We can understand these various dynamics by comparing to high-resolution equilibrium measurements [3] and employing a model where the electronic temperature changes on the ultrafast timescale throughout the Brillouin Zone. In future studies we hope to combine high-resolution trARPES with pump energy tunability to selectively probe the superconducting gap in greater detail.

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Ultrafast Surface and Bulk Carrier Dynamics in Photo-excited Topological Insulators

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ABSTRACT

Topological insulators have recently emerged as an intriguing class of materials and a highly-discussed topic of modern condensed matter physics. In particular, three-dimensional topological insulators exhibit a great attention because they possess a band gap in the bulk and conducting surface states. Their surface states are protected by time-reversal symmetry leading to a substantial suppression of back-scattering and to a robust helical spin texture. Such surface states in their simplest form can be viewed as Dirac fermions similar to that in graphene but without spin degeneracies. With such unique properties three-dimensional topological insulators have considered as milestones towards novel applications spanning from spin-based field-effect transistors to ultrafast optro-spintronic devices, whose performance depends strongly on the dynamics of excited carriers.

Using femtosecond time- and angle-resolved photoelectron spectroscopy we reveal the out-of-equilibrium dynamics of the binary, Bi_2Te_3, and the ternary, Bi_2Te_2Se, topological insulator [1-3]. We show that the interplay of surface and bulk transient carrier dynamics in a photo-excited topological insulator compound may alter the balance between electrons and holes in Dirac surface states. This can result to an unusually long-lived population of hot massless Dirac fermions following femtosecond optical photo-excitation.

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Non-equilibrium Momentum Dependent Dynamic of Unconventional Superconductors

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ABSTRACT

Understanding how superconductivity emerges from other competing phases and how this balance evolves through the phase diagram is one of the biggest challenges in the field of high Tc superconductors. By using high resolution time- and angle- resolved photoemission spectroscopy (tr-ARPES) we are able to directly probe the effects of optical excitation on the electronic structure of cuprate superconductors, and study the resulting quasiparticles, superconducting gap, and Cooper pair formation dynamics near their natural time- scales. Direct measurements of these and other non-equilibrium spectral phenomena through the phase diagram further illustrate the power of this unique time- and momentum-resolved spectroscopy. These results reveal new windows into the nature of the pairing interaction in high Tc superconductors.

Thermalization of Photo-excited Mott Insulators

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ABSTRACT

We use the nonequilibrium dynamical mean field formalism [1] to study the relaxation and thermalization of photo-doped carriers in Mott insulators. While the thermalization time depends exponentially on the gap size [2], the short-time relaxation in small-gap insulators can be significantly altered by impact ionization processes, if the pulse energy is high [3]. The relaxation of the carriers within the band is strongly affected by antiferromagnetic (short-range) order [4], and by phonon-scattering [5]. We also address the effect of dynamical screening of the photo-carriers [6] in models with long-range interactions.

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Combining Soft X-ray ARPES and STM with DFT and Many-body Correlations to Understand the Multiple Aspects of the Charge Density Wave in $TiSe_2$

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ABSTRACT

The transition-metal dichalcogenide *1T*-$TiSe_2$ is a quasi-two-dimensional (2D) layered material which undergoes a second order phase transition to a commensurate charge density wave (CDW) at $T_{CDW} \approx 200$ K. Since decades, theoretical and experimental works have been devoted to the study of the possible interplay between the CDW transition and electron-hole interactions. In particular, photoemission measurements of the hole-like valence-bands and electron-like conduction-band have been performed to target the bandstructure near the Fermi level since it determines the possibility for a BCS (in case of a semimetal) or a Bose-Einstein (in case of a semiconductor) type condensation of electron-hole pairs.

In the past ten years, *1T*-$TiSe_2$ has drawn a renewed interest due to the discovery of a superconducting phase and a proposed chiral-type CDW. Also, the quality of $TiSe_2$ crystals is strongly sensitive to the growth conditions since a small amount of defects or doping significantly changes macroscopic properties and interacts with the superconducting and CDW phases.

We theoretically show that electron-hole correlations strongly renormalize the electron spectral function near the Fermi level in such a way that the long-standing debate on the semimetallic or semiconducting character of the material finds a solution [1]. Our predictions agree with ARPES data.

We also study the consequences of chiral atomic displacements on the total energy using density functional theory and probe the 3-dimensional band dispersion using soft x-ray ARPES. Besides photoemission, we performed STM measurements to locally probe intrinsic defects and develop an understanding of their impact on the different aspects of $TiSe_2$ [2].

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Accessing the Self-energy of a Correlated Material with Time-resolved ARPES

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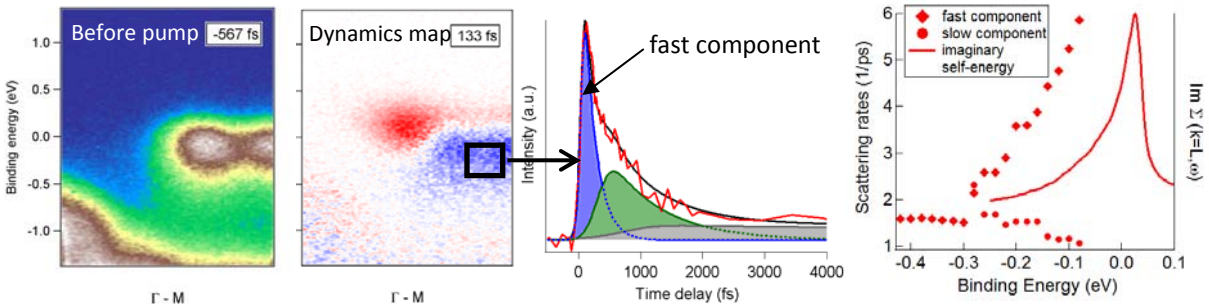
ABSTRACT

Transition metal dichalcogenides are a family of quasi-two dimensional materials, which have often been studied for their charge density wave (CDW) phases and more recently for applications in atomically thin electronics [1]. Among those, $TiSe_2$ offers a puzzling case, since the mechanism responsible for its CDW transition is still debated.

Here we present a time- and angle-resolved photoemission spectroscopy (trARPES) study of the charge density wave (CDW) phase of $TiSe_2$. trARPES measurements were performed at temperatures in the CDW phase and above the phase transition (T_c = 200 K), where CDW fluctuations are intense. Comparison of these two sets of data emphasizes that a similar mechanism is responsible for the suppression of the CDW phase [2] and its fluctuation phase. A detailed analysis of the recovery of these CDW fluctuations after photoexcitation reveals a slow and a fast component. The fast component, with a relaxation time of about 200 fs, shows unusual binding energy dependence. The corresponding scattering rate is compared to the imaginary part of a model self-energy [3]. This way, it is identified as the signature of strong electron-hole scattering, specific to the semi-metallic band structure of $TiSe_2$. We conclude that this electron-hole scattering drives the electronic instability leading to the CDW phase transition in $TiSe_2$.



Caption: *(left) trARPES data of $TiSe_2$ taken at 240 K at M point. (right) transient intensity of the CDW fluctuations and the scattering rate of the related slow and fast components compared to the model self-energy.*

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Superconducting Mechanisms of Iron-based and Cuprate Superconductors

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ABSTRACT

Two families of high temperature superconductors whose critical temperatures are higher than 50K are known at ambient pressure. One is the copper oxides and the other is the iron-based superconductors. Here we first present an overview of the ab initio numerical method developed for strongly correlated electron systems [1]. This muli-scale ab initio scheme for the correlated electrons is applied to an electron-doped iron-based superconductor LaFeAsO [2,3]. The superconductivity is reproduced in the variational Monte Carlo calculations in accordance with the experiments. The mechanism of the superconductivity is identified as enhanced uniform density fluctuations by one-to-one correspondence with the instability toward inhomogeneity (phase separation) driven by first-order antiferromagnetic (AF) and nematic transitions. The mechanism is analyzed in terms of the underlying orbital selective Mottness. Despite many differences, certain common features with the copper oxides are found. The emergence of the superconductivity in the copper oxides is further analyzed by the dynamical mean-field calculations [4]. From one-to-one correspondence of the gap function and the Green's function between the model for the cuprates and a simple two-component fermion model, we show evidence for the existence of hidden fermions that give birth to the strongly bound Cooper pairs. The hidden fermions survive even above Tc and generate the strange-metal pseudogap phase. A unified picture of these two striking results on iron-based and cuprate superconductors emerges in terms of localized-itinerant duality. We discuss possible interpretations of photoemission results in the light of our findings.

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Superconducting Instabilities, Spectral Functions and Quasiparticle Interference in Iron-based Superconductors

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ABSTRACT

We analyze and compare the structure of the pairing interaction and superconducting gaps in LiFeAs and Co-doped NaFeAs by using the ten-orbital tight-binding model, derived from ab initio LDA calculations with hopping parameters extracted from ARPES experiments. Using leading angular harmonic approximation to the multiorbital Hubbard model we analyze discuss the phase diagram and leading superconducting instabilities in both systems. We find four different configurations of the s-wave gap immediately below Tc: one in which the superconducting gap changes sign between two inner hole pockets and between the outer hole pocket and two electron pockets, one in which the gap changes sign between two electron pockets and three hole pockets, one in which the gap on the outer hole pocket differs in sign from the gaps on the other four pockets, and one in which the gaps on two inner hole pockets have one sign and the gaps on the outer hole pockets and on electron pockets have different sign. We discuss the phase diagram and experimental probes to determine the structure of the superconducting gap in LiFeAs. We argue that the state with opposite sign of the gaps on the two inner hole pockets has the best overlap with ARPES data. We also argue that at low T , the system may enter into a “mixed” s + is state, in which the phases of the gaps on different pockets differ by less than π and time-reversal symmetry is spontaneously broken. Using T-matrix approach we analyze how the superconducting state with opposite sign of the gaps on the two inner hole pockets in LiFeAs evolve upon changing the parameters towards NaFeAs compound, showing global s+- superconductivity where the gaps changes sign between all electron and all hole pockets

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High-energy Electronic Interaction in Iron-based Superconductors

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ABSTRACT

Recently we have observed a high-energy anomaly in angle-resolved photoemission spectra (ARPES) of iron-based superconductors, appearing in a form of kink in dispersion, stripe of spectral weight depletion, and abrupt increase of the scattering rate. We have shown that the well-known more than threefold band renormalization at the Fermi level is a part of the modification of the whole 3d iron band, induced by a strong high-energy electronic interaction. Similar high-energy features of the experimental spectrum have been found for many families of iron-arsenide and iron-selenide superconductors, including superconducting thin films. Matching ARPES experiment with results of dynamical mean field theory (DMFT) shows detailed agreement as for structure of the spectral function, implying that major deviations of these electronic systems from the one-electron model are to be attributed to the electronic correlations of the moderate strength. Interestingly, such anomalies are also common for the electronic spectra of cuprates and ruthenates, and are never found in ordinary electronic systems. Even for the materials, isostructural to iron superconductors, e.g. $SrPd_2Ge_2$ and $BaNi_2As_2$, the electronic spectrum is very close to the band structure calculations, the T_c is low and the superconductivity is believed to be of conventional BCS kind. This suggests that while there are so many differences between high-temperature superconductors inside iron-based family and even more between them and cuprates, there is a thing may unify and distinguish all unconventional superconductors.

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Tuning Electronic Correlations in Transition Metal Pnictides: Chemistry beyond the Valence Count

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ABSTRACT

The effects of electron-electron correlations on the low-energy electronic structure and their relationship with unconventional superconductivity are central aspects in the research on the iron-based pnictide superconductors [1, 2].

In this contribution, we emphasize the conceptual difference between the nominal valence count corresponding to the band filling and the effective orbital occupancies of the correlated states not only by doping but also by variations of the hybridisations. Soft X-ray angle-resolved photoemission spectroscopy (SX-ARPES) of different chemically substituted iron pnictides is combined with density functional theory (DFT) and dynamical mean-field theory (DMFT) calculations to show that the effective orbital occupancy of the correlated states is a more reliable tuning parameter for electronic correlations. Finally, the effective occupation-driven trend in the electronic correlation reported in our work supports the recently proposed connection between cuprate and pnictides phase diagrams [1, 3].

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ABSTRACTS

Tuesday, July 7th, 2015

CORPES15

Tuesday, July 7th

Chairpersons: S. Biermann, L. Patthey, P. Aebi, K. Matho

OC-EX-09	Charge order in cuprates: From hole to electron doping *A. Damascelli*
IT-EX-08	Resonant X-ray scattering of cuprates: Where inelastic and elastic meet *G. Ghiringhelli*
IT-TH-09	What does resonant inelastic X-ray scattering at the Cu L edge really measure? *K. Wohfeld*
OC-TH-10	Charge excitations in resonant inelastic X-ray scattering: Detecting enhanced small-momentum charge fluctuation of electron-doped cuprates *T. Tohyama*
IT-EX-10	Spin textures of polar and ferroelectric materials *H. Dil*
OC-TH-11	Metal-insulator transitions and magnetism in oxide interfaces *F. Lecherman*
OC-EX-12	Two dimensional electron gases at the (001) and (101) surfaces of TiO_2-anatase: Role of oxygen vacancies and UV-irradiation *P. Le Fèvre*
IT-EX-11	Fermi pockets and pseudogap in ligthly doped strontium iridates *A. Tamai*
IT-EX-12	Fermi arcs and their evolution in electron doped Sr_2IrO_4 *B.J. Kim*
OC-EX-13	Uncovering spin-polarised bulk electronic states in inversion-symmetric WSe_2 *J. Riley*
OC-TH-14	Nonempirical calculation of transition temperature for fulleride superconductivity *Y. Nomura*
IT-EX-13	Point node gap persisting beyond Tc in Bi2212 *T. Kondo*

Charge Order in Cuprates: From Hole to Electron Doping

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ABSTRACT

Charge ordering has resurged as a prominent phenomenon in the physics of high-T_c cuprates. In this talk I will review our recent results from Bi2201 [1,2] and YBCO hole-doped cuprates [3,4], as well as electron doped NCCO [5]. With the early discovery of stripe-like order in La-based cuprates, this establishes charge ordering instabilities to be omnipresent in all cuprate families. I will discuss the connection between charge ordering and pseudogap phenomenology [2,5], similarities and asymmetries between hole and electron doping [2,5], and the native local symmetry of charge modulations [3,4].

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Resonant X-ray Scattering of Cuprates: Where Inelastic and Elastic Meet

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ABSTRACT

The third decade of the saga on high Tc superconductors (HTS) based on copper and oxygen has been marked by important results obtained by resonant x-ray scattering (RXS), in particular in the soft x-ray regime where the Cu L_3 and the O K edges can be found. The development of better instruments at the synchrotron radiation beam lines has led to the demonstration that magnetic excitations can be studied with resonant inelastic x-ray scattering (RIXS), a crucial complement to the well-established inelastic neutron scattering technique[1,2]. RIXS has therefore been used to determine the dispersion relation of spin-flip excitations in several families of cuprates, revealing their persistence across the entire superconducting dome up to the strongly overdoped regime[3,4]. Somehow simultaneously the RXS experiments without energy resolution have been very effectively used to reveal charge order in striped cuprates. And after the discovery by RIXS of charge order also in YBCO[5], RXS has been very effectively used to characterize this elusive property of high Tc superconductors[6]. These results have consolidated the general picture where superconductivity in cuprates is mediated by spin fluctuations and develops around a quantum critical point characterized by charge density instabilities[7].

A new generation of instruments for RIXS is due to come into operation in the next 2-3 years. Energy resolution at Cu L_3 edge will break the symbolic barrier of 100 meV and reach the 30-50 meV range in routine operation. In 2015 ERIXS, at the new ID32 beam line of the ESRF, is becoming the first of those spectrometers to be available to users. Its novelty and strength is in the combination of unprecedented energy resolution and luminosity with a 6 degree-of-freedom sample manipulator (having the performances of a real diffractometer) and with a polarimeter allowing the simultaneous measurement of the energy and the polarization of the scattered photons. ERIXS will allow elastic, inelastic and standard RXS experiments in a variety of combinations, opening drastically new opportunities for a complete understanding of the resonant scattering experimental results.

I will present some recent RIXS results on 214 and 123 cuprates where the cross-talking between the inelastic and elastic components of the spectra is detected for the first time and provides crucial information on the effects of charge order on the low energy excitations[8,9].

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What Does Resonant Inelastic X-ray Scattering at the Cu *L* Edge Really Measure?

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ABSTRACT

Recent resonant inelastic x-ray scattering (RIXS) experiments at the Cu *L* edge of copper oxides suggest that this technique can be regarded as one of the best spectroscopic probes of the low energy excitations in the cuprates [1-10]. In this talk I would firstly give a brief and introductory overview of RIXS from a theoretical perspective. In particular, I will discuss: (i) the reason behind its recent success, (ii) challenges in modelling RIXS experiments, and (iii) the connection to other spectroscopies, including ARPES.

In the second part of the talk I would like to report our very recent, unpublished and to-be-submitted findings, which for the first time show in a completely unambiguous way what RIXS at the Cu *L* edge really measures in the cuprates. It will be shown that on a qualitative level: (i) in the so-called cross-polarized channel RIXS is sensitive to the spin dynamical structure factor (e.g. single magnons) whereas (ii) in the so-called parallel-polarized channel RIXS is mostly sensitive to the A1g projected charge dynamical structure factor, i.e. to both the charge excitations and to the two-spin excitations (e.g. bimagnons). However, a quantitative comparison between RIXS and these relatively simple structure factors is impossible. As a consequence, it will be suggested that the recently observed anisotropic softening of the RIXS spectra in the nodal direction of the superconducting cuprates [10] can simply be understood in terms of a RIXS « matrix-element » and not as following from the anisotropic softening of the magnetic excitations in the doped cuprates.

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Charge Excitations in Resonant Inelastic X-ray Scattering: Detecting Enhanced Small-momentum Charge Fluctuation of Electron-doped Cuprates

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ABSTRACT

Resonant inelastic x-ray scattering (RIXS) tuned for Cu L edge is a possible tool to detect momentum-dependent intra-orbital charge excitations in cuprate superconductors [1]. We theoretically investigate the possibility for observing the low-energy charge excitation with the same energy scale as spin excitation by RIXS [2]. We find that the core-hole Coulomb potential enhances the spectral weight of the charge excitation in electron-doped systems. Furthermore, from a large scale density-matrix renormalization group calculation, we find that electron-dopes system enhances small-momentum low-energy dynamical charge structure factor, whose energy is lower than that of spin excitation. This indicates a nontrivial mechanism of charge-spin coupling and superconductivity in electron-doped cuprates.

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Spin Textures of Polar and Ferroelectric Materials

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ABSTRACT

For spintronics applications nowadays mainly topological insulators are considered as important materials although many topological insulators are made up of technologically difficult materials. Furthermore, for most applications a tunable spin- and electronic structure is required, or in the ideal case the spin texture should be inverted. Tunable and technologically easily implemented materials are mostly found on the trivial side of the distinction of material classes. Although topological insulators might play a role in spintronics applications, we should not let trivial Rashba systems out of sight. In this respect especially materials with strong polar properties are expected to play an important role. Here we will give an overview of our recent results on the determination of the spin texture of several polar and even ferroelectric materials, both with 2D and 3D band structures. In these types of materials the Rashba-type spin splitting is expected to be enhanced due to the strong local electric fields. Furthermore, the sign of the spin helicity is predicted to be coupled to the local electronic polarization and can thus be switched by an external electric field.

The technological relevance of Rashba systems has previously been limited by the fact that any spin signal of the surface is overshadowed by spin degenerate bulk bands. Here we will show two approached to overcome this serious limitation. The first approach is based on the formation of a Rashba split 2DEG on a truly insulating substrate. By spin- and angle-resolved photoemission (SARPES) we have found that the 2DEG formed at the surface of bulk insulating $SrTiO_3$ shows a giant Rashba-type spin splitting [1]. Due to the presence of magnetic ordering a gap is opened at the Dirac point in this system and combined with the known superconductivity below 250 mK this could create a 2D platform for Majorana physics. It will be shown that the recipe for the formation of a surafce 2DEG can be extended to ferroelectric $BaTiO_3$.

The second approach to reduce the influence of spin degenerate bulk bands on the spin signal is to actually induce a similar spin splitting in these bulk states. In order to achieve this the inversion symmetry in the crystal has to be broken. It will be shown that for BiTeI and BiTeCl this results in a spindle torus shaped 3D Fermi surface [2] whereby in the latter we could for the first time follow the spin texture as a function of k_z [3]. Although highly polar, the spin structure in these materials can't be switched as it is intrinsically coupled to the atomic stacking order. To achieve such a switching a ferroelectric materials is needed. Here it will be shown that thin GeTe films are ferroelectric and that both the bulk and surface states of this material exhibit a Rashba-type spin splitting which is directly coupled to the ferroelectric polarization [4].

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Metal-insulator Transitions and Magnetism in Oxide Interfaces

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ABSTRACT

Recent advances in designing materials beyond nature's original conception open a fascinating new chapter in condensed matter physics. Novel compounds and structurings, e.g. in the field of oxide heterostructures, are thereby often subject to strong electron correlation [1]. Realistic theoretical schemes beyond conventional density functional theory (DFT) as well as static correlation methods such as DFT+U are needed to account for the competition between localization and itinerancy in these challenging materials.

We here present an elaborate methodology to tackle the many-body effects in oxide interfaces on a realistic level. By means of the advanced combination of DFT with explicit many-body techniques such as dynamical mean-field theory it becomes possible to address the intricate interplay between band-structure and electronic correlations even in complex architectures [2,3].

New insight into the metallicity and the key mechanisms for itinerant ferromagnetism at the $LaAlO_3/SrTiO_3$ interface will be provided. The interplay of oxygen vacancies and electronic correlations for establishing magnetic order at different defect concentrations is discussed. Double-exchange physics with a relevant Hund's J_H competes with the order of local moments. Furthermore we study the puzzling physics at different Mott-band insulating interfaces based on $GdTiO_3/SrTiO_3$,, i.e. along [001], [110] and [111]. Layer-dependent Multi-orbital metal-insulator transitions and ordering instabilities are revealed. An outlook towards the investigation of out-of-equilibrium physics in such demanding correlated materials is provided.

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Two Dimensional Electron Gases at the (001) and (101) Surfaces of TiO_2-anatase – Role of Oxygen Vacancies and UV-irradiation

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ABSTRACT

The study of two-dimensional electron gases (2DEGs) in TMO surfaces/interfaces has become a very active field of research. The archetypal example, $SrTiO_3$-based heterostructures, display many fundamentally interesting properties[1], such as field-effect induced insulator-to-superconductor transitions, magnetism and the coexistence of magnetism and superconductivity. More recently, the discoveries of 2DEGs at the bare (001), (110) and (111) surfaces of $SrTiO_3$[2] and $KTaO_3$[3] triggered new avenues of research.

We report here the existence of metallic two dimensional electron gases (2DEGs) at the (001) and (101) surfaces of bulk insulating TiO_2-anatase due to local chemical doping by oxygen vacancies in the near-surface region. Using angle-resolved photoemission spectroscopy, we find that the electronic structure at both surfaces is composed of two occupied subbands of d_{xy} orbital character. While the Fermi surface observed at the (001) termination is isotropic, the 2DEG at the (101) termination is anisotropic and shows a charge carrier density three times larger than at the (001) surface. Moreover, we demonstrate that intense UV synchrotron radiation can alter the electronic structure and stoichiometry of the surface up to the complete disappearance of the 2DEG. These results open a route for the nano-engineering of confined electronic states and the control of their metallic or insulating nature using UV illumination at different surfaces of anatase.

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Fermi Pockets and Pseudogap in Ligthly Doped Strontium Iridates

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ABSTRACT

The 5*d* transition metal iridium oxides may host exotic quantum phases emerging from the interplay of correlations and strong spin-orbit coupling [1,2]. Iridates of the Ruddlesden-Popper series $Sr_{n+1}Ir_nO_{3n+1}$ share key structural, magnetic and electronic properties [3] with the parent compounds of copper oxide superconductors and are thus of particular interest as candidate materials for engineering unconventional superconductivity.
Here, we present the electron doping evolution of $(Sr_{1-x}La_x)_2IrO_4$ and $(Sr_{1-x}La_x)_3Ir_2O_7$ by angle-resolved photoemission. In the single layer $(Sr_{1-x}La_x)_2IrO_4$, metallicity emerges from a rapid collapse of the Mott gap with doping rather than from a gradual spectral weight transfer as observed in cuprates [4]. At the highest doping level of x=0.05, we find a large circular Fermi surface centered at Γ with nodal quasiparticles and an antinodal pseudogap. Because of the structural reconstruction of the IrO_2 plane, the band structure is back folded into a small Brillouin zone and gapped Fermi pockets rather than Fermi arcs [5] are observed.
In the bilayer $(Sr_{1-x}La_x)_3Ir_2O_7$ the doping evolution is fundamentally different [6]. Concomitant with the metal-insulator transition around $x \approx 0.05$ we find the emergence of coherent quasiparticle states forming a closed small Fermi surface of volume 3x/2, where x is the independently measured La concentration. The quasiparticle weight *Z* remains large along the entire Fermi surface, consistent with the moderate renormalization of the low-energy dispersion, and no pseudogap is observed.

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Fermi Arcs and their Evolution in Electron Doped Sr_2IrO_4

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ABSTRACT

The physical origin of the pseudogap and its relation to the superconducting gap in high temperature superconducting cuprates remain highly controversial. In this talk, I will show that this unique cuprate physics can be studied on a novel material platform, a 5*d* transition-metal oxide Sr_2IrO_4, which effectively realizes a spin one-half Heisenberg antiferromagnet on a square lattice[1,2]. Through in situ surface electron doping, we have recently shown that angle-resolved photoemission spectra (ARPES) of Sr_2IrO_4 display Fermi arcs and an 'antinodal' gap, which evolve as a function of doping and temperature in strong parallel to those observed in the cuprates[3]. However, because doping is limited to the sample surface, the insulating nature of the bulk limits low-temperature study using ARPES. I will discuss how our materials strategy circumvents this problem and reveals the entire phase diagram of electron doped Sr_2IrO_4. We find that the parallel between cuprates and iridates holds down to the lowest temperature, pointing to a common origin of the pseudogap in the two microscopically disparate systems. We conclude that the pseudogap is a generic feature of a correlated electron fluid that has a *d*-wave instability.

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Uncovering Spin-polarised Bulk Electronic States in Inversion-symmetric WSe_2

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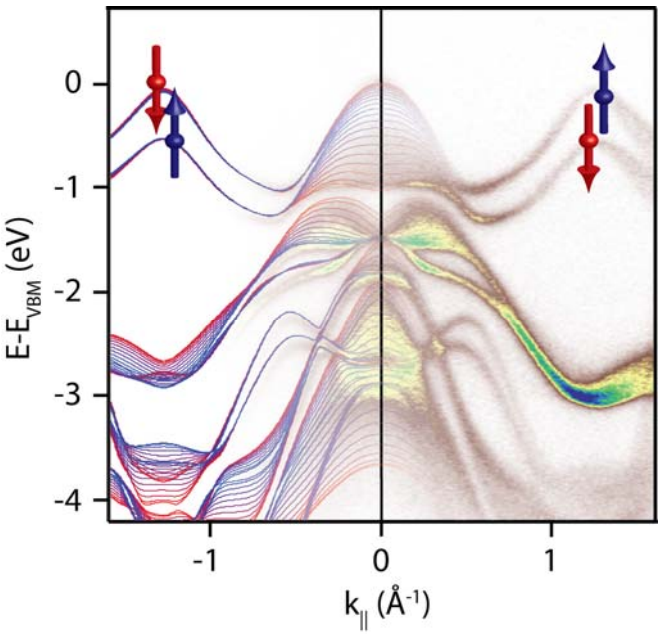
ABSTRACT

Stabilising spin-polarised electronic states without magnetism is strongly desired to enable all-electrical control of electron spins, underpinning a myriad of future applications in spintronics. It is generally accepted that this requires the breaking of global structural inversion symmetry; however, here we present direct evidence from spin- and angle-resolved photoemission spectroscopy that bulk states in the inversion-symmetric transition-metal dichalcogenide WSe_2 are strongly spin polarized [1]. We show how this arises due to local symmetry breaking within the individual structural components that make up the unit cell of this compound. Our study provides a direct experimental observation of a recently predicted `hidden' spin polarisation in centrosymmetric materials [2]. Moreover, exploiting photoelectron interference effects, our photon energy-dependent measurements reveal how the spin polarization switches sign for states localised in neighbouring layers of the crystal, providing a visualisation of the locking of the spin with valley and layer pseudospins [3] in transition-metal dichalcogenides. Control of the layer pseudospin could bring new opportunities for stabilising large and directly tunable spin splittings in solids, opening new potential for exploiting hidden spin polarisations to create improved spintronic materials,



Valence band dispersions of WSe_2 measured by angle-resolved photoemission, showing excellent agreement with theoretical calculations of the k_z-dependent bulk electronic structure (coloured lines). The spin texture measured at the K & K' points of the Brillouin zone is shown schematically by coloured arrows.

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Nonempirical Calculation of Transition Temperature for Fulleride Superconductivity

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ABSTRACT

The alkali-doped fullerides A_3C_{60} (A = K, Rb, and Cs) show a unique phase diagram, in which the high transition-temperature (T_c) *s*-wave superconductivity emerges next to the Mott-insulating phase [1]. The existence of the Mott phase indicates that A_3C_{60} is a strongly correlated material. On the other hand, the observed low-spin state [1] and the dynamical Jahn-Teller effect [1] in the Mott insulating phase suggest that electron-phonon interactions also play a significant role.

In the present study, we aim at (i) a unified understanding of the phase diagram and (ii) a calculation of T_c without employing any empirical parameter. For these purposes, it is essential to take care of the subtle interplay between the Coulomb and electron-phonon interactions.

In order to take account of these interactions quantitatively, we employ an extension of DFT+DMFT (density functional theory + dynamical mean-field theory). We apply a recently formulated *ab initio* downfolding scheme for electron-phonon coupled systems [2] to fcc A_3C_{60} systems. Then, we construct realistic low-energy Hamiltonians consisting of the electron transfer, the Coulomb interaction and the phonon-related terms. We show nonempirically that the Jahn-Teller phonons dominate over the Hund's coupling, which leads to effectively negative exchange and pair-hopping interactions.

The derived multi-orbital Hamiltonians are analyzed by means of the extended DMFT. The results comprehensively reproduce the experimental phase diagram including the *s*-wave superconductivity and low-spin Mott-insulating phase. Remarkably, the calculated maximum T_c of ~ 28 K is in good agreement with the experimental result (35 K). A detailed analysis on the superconducting mechanism reveals that the strong electron correlations and the Jahn-Teller phonons cooperate in driving the *s*-wave superconductivity [3]. Applications of the present scheme to other strongly correlated unconventional superconductors are important and interesting future issues.

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Point Node Gap Persisting beyond T_c in Bi2212

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ABSTRACT

In cuprates, the energy gap (pseudogap) starts opening at a temperature much higher than T_c, in some cases above the room temperature. Many experimental evidences point to a competing-order origin, rather than the preformed pair, for the pseudogap observed around the antinode. On the other hand, the energy gap near the node is expected to open due to the electron pairing as it is free from a contamination by the competing order establishing around the antinode. Unveiling the nature of the spectral gap near the node is therefore crucial to elucidate the superconducting mechanism in cuprates. A difficulty however is the small magnitude of the gap, which has been challenging the experimentalists to investigate.

It has been proposed that the pairing-gap evolution with temperature simply follows the conventional BCS function, and Fermi arcs emerge at T_c, marking momentum borders between the superconducting and the competing pseudogap regions [1]. In contrast, a contrasting view was recently proposed [2,3]: its underlying idea is that one should discard the notion of electron quasiparticles, instead pay attention to the density of states, which is an effective way of judging the existence of energy gap. Accordingly a momentum integration of angle-resolved photoemission spectroscopy (ARPES) spectra has been performed over a selected part of the momentum space. This quantity contributed from the nodal region was found to have a gap-like structure even above T_c. To address the controversial issue, we use a laser ARPES capable of an ultra-high energy resolution and a bulk-sensitivity, and provide a missing evidence for a single-particle gap near the node, signifying the point-node gap state persistent way above T_c in $Bi_2Sr_2CaCu_2O_{8+d}$.

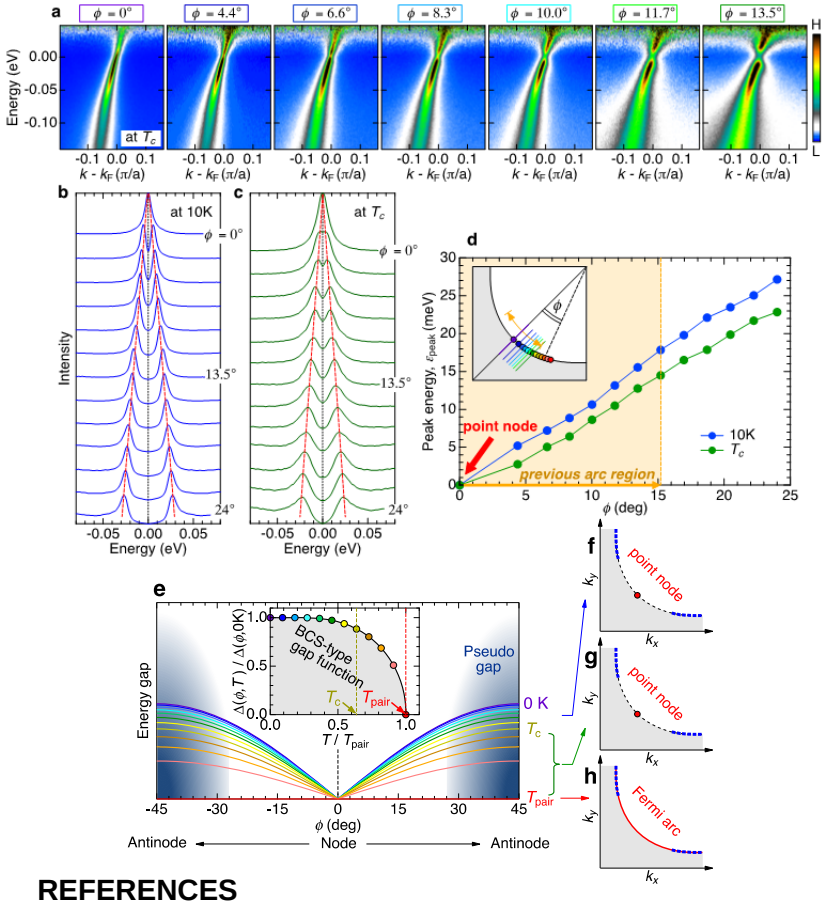

Figure: (**a**) Dispersion maps at T_c along several momentum cuts (color lines in the inset of (**d**)). Each map is divided by the Fermi function at the measured temperature. The described ϕ is the direction of k_F point (defined in the inset of (**d**)). (**b**) Symmetrized EDCs at k_F over a wide range of ϕ (circles in the inset of (**d**)) at 10K and T_c (=92K), respectively. (**d**) Fermi angle ϕ dependence of spectral peak energies, ε_{peak} (10K) and ε_{peak} (T_c), determined from the data in (**b**) and (**c**), respectively. The inset indicates the measured momentum space with the Fermi surface. (**e**) Schematic behavior of energy gap summarized based on our ARPES results. Temperature evolution of point-node gap state with a BCS-type temperature dependence (inset curve) is depicted for all directions (ϕs). Temperatures for each curve are indicated in the inset panel with colored circles. (**f,g**) The gapped Fermi surface with a point node persists beyond T_c up to the temperature of pair formation (T_{pair}). (**h**) Emergence of the gapless Fermi arc due to the pseudogap around the antinode (blue dotted curves) is described.

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POSTER SESSION I

Tuesday, July 7th, 2015

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PO-I-EX-04	Spin-selectivity in resonant ARPES from spin-momentum locked surface states *H. Bentmann*
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G. Liu

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J. Lobo-Checa

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H. Maaß

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G. Manzoni

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A.S. Mishchenko

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B. Moritz

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L. Nicolaï

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R. Rausch

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A. Ribak

PO-I-EX-28 Self-organization of Bi on InAs(1 1 1)
C. Richter

PO-I-EX-29 Probing the geometric and electronic structure of the surface of the topological insulator $TlBiSe_2$
E.F. Schwier

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PO-I-EX-32 Momentum microscopy of Ni-intercalated layered semiconductor TiS_2
S. Suga

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A. Tejeda

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C. Varma

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I. Vobornik

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PO-I-EX-38 The quantum materials spectroscopy center at the Canadian light source
S. Zhdanovich

Gap or no Gap? The Effects of Disorder and Defects on the Band Structure of Graphene

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ABSTRACT

Graphene presents high potential for providing the next generation of electronic materials due to its strictly two-dimensional character as well as its high electron mobility. Among the remaining challenges is the question whether or not a gap can be opened at the Dirac point in the electronic structure. In principle, there are a number of mechanisms that induce a band gap opening at the Dirac point, such as lifting the sublattice symmetry or enhancing the effective spin-orbit interaction in graphene. However, the effects of disorder and defects on the electronic structure of graphene have to be considered, in particular when adatoms are deposited onto the graphene layer, which themselves introduce disorder into the system.

Using angular resolved photoemission spectroscopy, we show that depositing thallium atoms onto epitaxial graphene on SiC induces both short-range and long-range scattering, which strongly affects the graphene band structure. As the line width broadening is much larger than the predicted gap opening due to enhanced spin-orbit coupling from the deposited thallium atoms, the gap will be masked by the induced disorder.

On more general grounds, using a simple real-space tight-binding model, we present the effects of disorder and defects on the band structure of graphene in momentum space near the Dirac point. While all calculated defects strongly alter the band dispersion and line width near the Dirac point, only one randomly extracted atom from the same sublattice will open an actual band gap. All other defects, that have been considered, either generally preserve the conical band dispersion or open an apparent band gap with strongly broadened, but not entirely delocalized, states within the apparent gap. These findings bear great resemblance to the “elongated” Dirac points that have been experimentally found by photoemission spectroscopy and discussed extensively in the literature. We surmise that these elongated Dirac points are at least in part due to specific defects at the surface.

We conclude that disorder and defects mask the opening of a real gap, which has to be considered when designing the graphene band structure.

Uncertainty Principle for Experimental Probes: Fast Spectroscopy vs. Slow Microscopy

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ABSTRACT

The result of a physical measurement depends on the timescale of the experimental probe: this is one of the major teachings of quantum mechanics in the first half of the 20th century. In solid-state systems, this simple quantum mechanical principle can have far-reaching consequences: the interplay of several degrees of freedom – for instance close to charge, spin or orbital instabilities – combined with the disparity of the timescales associated to their fluctuations can lead to seemingly contradictory interpretations of experimental data.

This is the case for systems of adatoms adsorbed on semiconductor surfaces where different experiments suggest different ordering phenomena. Using most recent many-body theoretical techniques including the self-consistent combination of the GW approximation with Dynamical Mean-Field Theory,[1] we analyze the experimental data and develop a coherent theoretical picture of the associated fluctuations.[2] Our work reconciles angle-resolved photoemission data, scanning tunneling microscopy and core-level spectroscopy, and presents a first principles many-body description for each of them.

Furthermore, investigating the role of temperature-dependent screening processes in surface systems, we show that temperature can drive insulator-to-metal transitions, thus giving a theoretical account of hitherto unexplained experimental observations.[3]

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Evidence for Coupled Spin-orbital Texture in Rashba Spin-split BiTeI

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ABSTRACT

In materials with broken inversion symmetry, the electron spin degeneracy can be lifted by spin-orbit interactions, often through a so-called Rashba effect. This is seen as a linear splitting of the bands in momentum, producing concentric spin-chiral bands at constant energy. BiTeI has recently been shown to host a giant Rashba splitting within its bulk band structure, which is inherited by states at its surface, thought to be well described by a Rashba model [1]. Through photon energy and polarisation-dependent angle-resolved photoemission measurements, we show that these spin-split branches additionally develop disparate orbital textures. Building on recent work on topological insulators [2], our measurements show in-plane orbital texture switches from being tangentially aligned to the constant energy contours, to a radial alignment, at precisely the Kramer's degenerate point. By exploiting resonant enhancements, we are able to selectively tune between orbital textures arising from different atomic species, which we support with density functional theory calculations, and assuming a layer-by-layer interference of the underlying wavefunction [3]. Together with circular dichroic measurements highlighting a possible out-of-plane spin canting, this demonstrates a rich coupling of the atomic, orbital and spin degrees of freedom. This level of control presents exciting new opportunities for orbital engineering of spin splitting in strong spin orbit systems for potential spintronic applications.

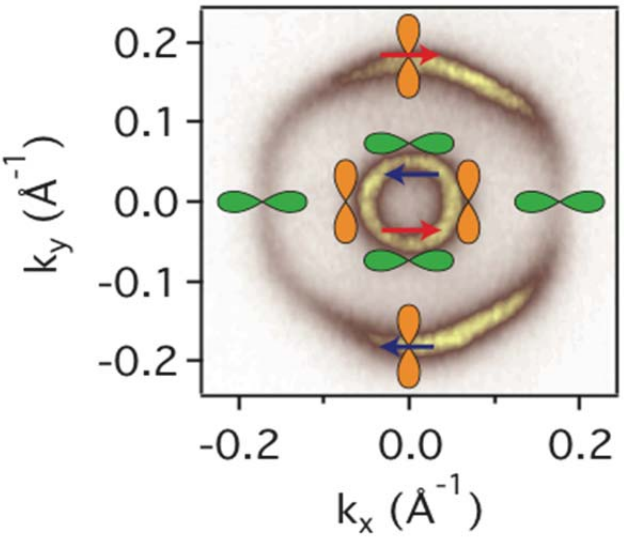

Fig. 1: Angle resolved photoemission measurements at the Fermi surface of BiTeI with imposed spin and orbital schematic, highlighting the disparate orbital textures of the concentric bands.

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Spin-selectivity in Resonant ARPES from Spin-momentum Locked Surface States

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ABSTRACT

Resonant photoemission has been widely applied as an element- and orbital-selective probe of electronic valence states in solids. It is based on the interference between the direct photoemission channel and intermediate core-excited states that reach the same final state via autoionization and emission of an Auger electron [1].

In this contribution we report on resonant angle-resolved photoemission (ARPES) experiments on epitaxially grown Bi/Ag(111) [2,3]. The large spin-orbit coupling in this system gives rise to spin-momentum locked surface states, where states with opposite momentum carry opposite spin (Rashba effect). Pronounced modulations in the photoemission intensity of these Bi 6p derived surface states are observed as the photon energy is tuned through the Bi 5d absorption edge. In particular, a complete suppression of spectral weight occurs shortly below the core level excitation energy, a characteristic signature of interference in the resonant photoemission process [1]. Interestingly, the observed effect is highly spin-selective in the sense that interference for spin-up and spin-down valence states is only observed at the Bi $5d_{5/2}$ and the $5d_{3/2}$ core excitations, respectively. Based on a simple model we attribute this spin selectivity to the distinct spin configurations of the Bi $5d_{5/2}$ and $5d_{3/2}$ core holes.

Our results establish a new spin-selective effect in resonant photoemission from spin-momentum locked surface states that—in particular when combined with the element-specifity of the process—may proof useful for a variety of other material systems.

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A Green's Function Approach to Orbital Polarons in $KCuF_3$

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ABSTRACT

Hole doping of a Mott or charge-transfer insulator with magnetic and orbital order in the ground state [1] poses numerous challenging questions. We present a variational solution of the spectral properties of a single charge (hole) doped into a superexchange model which describes interacting spin S=1/2 and orbital e_g degrees of freedom at Cu^{2+} ions [2] and is designed to represent the physics behind $KCuF_3$. The problem is approached by generating the equations of motion for the Green's function by means of subsequent Dyson expansions, up to a certain degree of interaction [3]. The resulting set of equations is then solved as a linear system, yielding the different Green's functions. We then compare this method to the Self Consistent Born Approximation (SCBA), successfully used before to study the problem in question [4]. We find that our method gives a very similar result for the ground state, although it can be argued that it is both more dependable as well as more flexible, owing to the fact that it is a systematic expansion allowing one to carefully choose the leading terms as well as to take into account the real-space constraints coming from the exclusion of double-occupancy states. The present method provides microscopic insights into the mechanism of hole propagation and could be easily applied to other models, especially in polaron research.

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Electron Dynamics in Graphene by Ultrafast Tr-ARPES

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ABSTRACT

Graphene's electronic and optical properties are intrinsically governed by the conical dispersion of the π-bands localized at the K-point far from the Brillouin zone centre. Ultrashort pulses of high energy photons (>20 eV) are required to explore the electronic dynamics in the Dirac cone. Artemis is a user facility offering an ultrafast XUV beamline and a photoemission end-station for Time- and Angle- Resolved PhotoEmission Spectroscopy (tr-ARPES) with mid-IR pumping. High Harmonic Generation in gas gives access to photons in the energy region from 16 eV to 80 eV with a time resolution of 30 fs at 1 kHz repetition rate [1]. Here we present an overview of different tr-ARPES studies on hot carrier dynamics in graphene.

A quasi-free-standing monolayer of graphene (MLG) is optically pumped with a ~30 fs IR pulse. Within the excitation pulse duration, electron-electron interactions lead to the formation of a thermalized distribution of hot carriers [2]. The contribution of optical and acoustic phonons in the cooling of the electronic temperature is measured by tr-ARPES and leads to the conclusion that supercollisions play a key role in the slow recovery [3]. A large carrier multiplication factor is observed for n-doped graphene [4], showing that the Dirac carrier dynamics can be controlled by tuning the doping level. In an independent study with a direct interband excitation regime and sufficient pumping fluence we observe a population inversion across the Dirac point [5-6]. This excited state persists over 130 fs supporting the potential of graphene for applications in THz amplification.

AB-stacked bilayer graphene (BLG) on a substrate is predicted to open a small band gap at the Dirac point with great importance for electronic device applications. Such a gap gives rise to a bottleneck in the decay of hot carriers and results in an accumulation of charge at the bottom of the conduction band. Indeed the comparison between BLG and MLG reveals different relaxation times supporting the presence of a band gap [7]. Complementarily, the band structure of BLG can be controlled in an out-of-equilibrium state by exciting the BLG E1u lattice vibration. At resonance excitation (6.3 μm pump wavelength) the peak electronic temperature and cooling time are significantly reduced [8]. Based on DFT frozen phonon calculations it is confirmed that this anomalous dynamics corresponds to the modification of a gap structure at the Dirac point.

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Anomalous Spectral Features of a Neutral Bilayer Graphene

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ABSTRACT

Graphene and its bilayer are two-dimensional systems predicted to show exciting many-body effects near the neutrality point. Previous angle-resolved photoemission spectroscopy (ARPES) measurements have focused on epitaxial graphene grown by heating the silicon carbide crystal, but the electronic structure of epitaxial graphene is easily affected by a strong interaction with the substrate[1,2]. In this work, we report the first high resolution ARPES measurements on undoped exfoliated bilayer graphene (ExBLG). Graphene samples were prepared by conventional micro-mechanical cleavage method on heavily n-doped Si substrates with native oxide only. Raman spectroscopy was used to determine the number of graphene layers and sample location. Various photon energies were chosen to enhance the photoemission intensity of higher or lower π bands and the electronic structure of ExBLG were compared with the result of SiC substrate. The band mapping of ExBLG is obtained with Fermi level residing around the Dirac point, indicating that the ExBLG is charge neutral. The tight-binding method was utilized to calculate the electronic structure of graphene and could be fitted well with the experimental data. We also found two essential aspects of its many-body physics: the electron-phonon scattering rate has an anisotropic k-dependence and the type of electronic liquid is non-Fermi liquid. The latter behavior is evident from an observed electron-electron scattering rate that scales linearly with energy from 100 meV to 600 meV and that is associated with the proximity of bilayer graphene to a two-dimensional quantum critical point of competing orders[3,4].

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Surface and Bulk States Scattering Mechanisms in Topological Insulators

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ABSTRACT

The first observation of a persistent electron population in the photo-excited spin helical surface state of topological insulators (TIs) has gathered an increasing attention on the out-of-equilibrium electronic properties of these materials [1-7]. In particular, the aim is to enhance the surface spin transport properties circumventing the limitation of the bulk transport. Hence, a deep understanding of the scattering mechanisms between the surface and bulk states of TIs is a key issue. The electron-phonon scattering was initially proposed as the most relevant mechanism responsible for the relaxation dynamics of the photo-excited electrons [1, 2]. However, a more complex picture emerges from our recent time resolved ARPES experiments on a wide set of TIs, displaying a broad range of n-doping (Bi_2Se_3, $GeBi_2Te_4$) and p- doping (Bi_2Te_3, $GeBi_2Te_4$, Sb_2Te_3, Sb_2Te). The different dynamics observed in the bulk and surface states of p-doped Bi_2Te_3 and $GeBi_2Te_4$ suggest that charge diffusion is also at play. Furthermore, the role of the sub-surface charge diffusion has been recently proposed on the base of the asymmetry in the electron-hole dynamics in n- and p- doped TIs [5]. However, when the hole doping is increased even more, as in the case of heavily p-doped Sb_2Te_3 and Sb_2Te, the electron dynamics in the surface states becomes faster than for Bi_2Te_3 and comparable to n-doped Bi_2Se_3. Furthermore, in contrast to p-doped Bi_2Te_3, in the case of heavily p-doped Sb_2Te_3, the dynamics in the surface and bulk states are the same, thus indicating a strong coupling between the two. This apparently conflicting behavior between n-doped Sb_2Te_3, p-doped Bi_2Te_3 and heavily p-doped Sb_2Te_3 might suggest that other sources of scattering, as for example impurities, are influencing the relaxation dynamics in TIs [6].

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Quasi-1D Band Dispersion and Metallization in Long Range Ordered Graphene Nanoribbons

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ABSTRACT

Graphene-like 2D organic materials can be grown and confined onto suitable surfaces depositing and activating selected molecules with different strategies in order to be employed as active media in organic electronics devices. In this respect, the surface-confined polymerization is a very promising bottom-up approach that allows the creation of layers with desired architectures and tunable optical or electronic properties. The most successful method used to obtain ordered polymers on surfaces in ultra-high vacuum is based on the Ullmann coupling reaction, producing covalently linked networks starting from aryl halide precursor molecules [1,2]. A surface-catalyzed dehalogenative polymerization has been recently evidenced for the (1,4)-dibromobenzene (DBB)/Cu(110) interface coupling structural and spectroscopic measurements [3]. In the submonolayer range, an organometallic phase is obtained for room-T deposition evolving into planar one dimensional polymeric structures of n=3 armchair graphene nanoribbons (3-AGNRs) above 200°C. Therefore, we have investigated the structural and electronic properties of (DBB,DIB)/Cu(110) interfaces in the submonolayer range combining LEED, STM/STS, HR-XPS and ARPES measurements on the CASSIOPEE beamline. On the one hand, ARPES intensity maps allowed us to identify a quasi-one dimensional graphene-like π-band as a consequence of the polymerization process with a direct HOMO-LUMO band gap of 1.15 eV and a metallic character [4]. On the other hand, STS local conductance maps evidence confinement of LUMO states for short oligomers above the Fermi level, decreasing below the Fermi level for “long” polymers in agreement with ARPES data. The metallic character is shown to originate from a substantial substrate/polymer interaction well described by our DFT calculations. These results will be discussed in the general context of organic/inorganic interfaces. The perspective of engineering the gap in graphene nanoribbons is known as a feasible route towards future c-based nanoelectronics.

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Writing on Topological Insulators

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ABSTRACT

3D topological insulators (TIs) are a novel class of materials with an insulating bulk and metallic surfaces [1]. The remarkable properties of TIs and their high potential for a wide range of applications ranging from spintronics to quantum computation are due to the existence of two-dimensional - topologically-protected - electronic states on their surface. Enormous scientific effort is invested to generate situations in which these topological surface states dominate the physical response of the system.

With a view to making topological surface states the dominant source of conductivity, our works investigates the possibility to exclude bulk-related electronic states from the Fermi level of TIs. Using Angle-Resolved PhotoElectron Spectroscopy I will show that this is possible at pre-defined sample locations by the interplay of an intense ultraviolet photon beam and band-bending effects

In other words, I will describe how to “write” small - micro-metric - letters on a topological insulator [2].

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Investigating Quasiparticle States at Metal/Organic Interfaces by Angle-resolved Photoemission

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ABSTRACT

Metal-organic interfaces play a crucial role for the electronic functionality and overall performance of organic devices. Such interfaces furthermore provide an interesting playground to study fundamental physical effects such as interaction mechanisms and their influence on the electronic structure.

In case of particular adsorbate/substrate combinations the lowest unoccupied molecular orbital (LUMO) is (partially) occupied due to hybridization with and charge transfer from the metal substrate [1]. Using high-resolution photoelectron spectroscopy (PES), for some systems (amongst them phthalocyanines (Pc) and 1,4,5,8-naphtalene tetracarboxylic dianhydride (NTCDA) on metall surfaces) a peculiar, very narrow feature can be observed at the Fermi energy, whose origin is believed to be a consequence of strong electronic correlations between molecular states and the Bloch states of the substrate [2]. At low temperatures (T < 20K), the line-width of this feature amounts to only ~ 10 meV, representing an unusually small energy scale for electronic excitations in these systems. Moreover, the signal displays strong temperature dependence and is directly connected to the binding energy of the LUMO.

By additional angle resolved PES experiments using a high-resolution momentum microscope that allows us to image the complete reciprocal space distribution of photoelectrons simultaneously, we intend to shed light on the particular nature of this quasiparticle feature at the Fermi energy. First results for NTCDA/Ag(111) show that the involved quasiparticle state and the LUMO reveal no differences of spectral weight in reciprocal space, thus indicating identical symmetries. Moreover, we observe similarity to e.g. Cerium systems, in which the intensity of the Kondo resonance in k-space is strongly enhanced, where a conduction band crosses the Fermi energy [3].

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Luttinger Parameters of the Metallic Boron Doped Diamond Determined by ARPES

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ABSTRACT

By doping the pure diamond with boron atoms, a transition towards a metallic phase takes place for a boron concentration larger than 3 x 10^{20} at./cm^3 [1]. This metal-insulator transition is accompanied by the appearance of superconductivity, with a critical temperature below 4 K [2].

Performed on (100) - oriented epilayers, the electronic band structure of the metallic phase has been investigated at low temperature by ARPES, in several directions of the reciprocal space. Using photons with tunable energy provided by the synchrotron Soleil source, the band structure of this three dimensional material has been measured along the high-symmetry directions (100) and (110) but also out of these directions.

The evolution of the band structure, recorded in the second and third Brillouin zones, is analyzed in relation with its position in the reciprocal space. Experimental bands are compared with theoretical ones, calculated for the pure diamond using the DFT or the k.p model. This analytical k.p model, developed to describe the band tops of semi-conductors, leads us to characterize the metallic diamond with a unique set of Luttinger parameters. These experimental parameters corroborate the parameter values calculated for the pure diamond by some theoretical groups [3], but are slightly different from the values extracted from cyclotron resonance experiments.

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Theoretical Study for the Well Screened State in Core-level X-ray Photoemission Spectroscopy for Transition Metal Compounds

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ABSTRACT

Core-level X-ray photoemission spectroscopy (XPS) is a powerful and unique tool to study electronic states of strongly correlated electron systems, such as 3d transition metal compounds. Owing to recent experimental progresses, especially in energy resolution and bulk sensitivity, spectral fine features have become observed in main lines of transition metal 2pXPS for various 3d compounds. As an example, in the Mn 2pXPS of $LaMnO_3$ (LMO) and $La_{1-x}Sr_xMnO_3$ (LSMO), temperature and carrier-doping dependent main-line structure has been reported. [1] The main-line structure is expected to reflect valence states near Fermi energy E_F, and has attracted much attention in connection with the electronic state related with colossal magnetoresistance and rich phase diagram of LMO and LSMO. The main-line structure reflects well-screened final states, where the so-called nonlocal charge screening from the neighboring MnO_6 unit toward the core-excited Mn site plays a key role. The nonlocal screening (NLS) effect, which was first pointed out by M. A. van Veenendaal and G. A. Sawatzky [2], is beyond description of a simple single impurity model conventionally used to analyze 2pXPS spectra. Thus, a development of a theoretical framework is required.

In this context, we developed recently a new framework considering the dynamical mean-field under realistic crystal structure in order to investigate the NLS effect on NiO and cuprates.[3] In the framework, the correlated 3d band is effectively mapped into the single impurity Anderson model, and the NLS is represented as the charge screening from the 3d band. Thus, a plausible description for the well screened states of 2pXPS including the NLS process is available.

In this study, we apply the framework to investigate the nature of the well screened state in 2pXPS for LSMO and undoped $LaMnO_3$. In LMO, we show that the NLS is directly reflecting the C-type orbital ordering, which plays an essential role for the formation of the main-line shoulder structure of the Mn 2pXPS observed in experiments. On the other hand, in hole-doped LSMO, we show that ferromagnetism and metallicity, which are related with the double exchange mechanism, play the key role for the formation of the pronounced peak in the Mn 2pXPS main line. In this session, we will compare the nature of the NLS in LMO and LSMO with the ones in other 3d compounds such as $LaCoO_3$ and NiO, and discuss the systematics in NLS, such as the spin and orbital selectivity, which reflects the spin and orbital character of valence states near E_F.

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Resonant Inelastic X-ray Scattering with Extreme Ultraviolet Source

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ABSTRACT

Resonant inelastic X-ray scattering (RIXS) is a powerful technique for studying the low energy excitations of many-body materials, which carry the rich information about the interaction between charge, orbital and spin degrees of freedom. RIXS at the extreme ultraviolet energy can achieve superior energy resolution comparable to the thermal energy scale (~ 20 meV). In this poster we will present results at EUV regime where *dd*, *ff* and other low energy excitations can be revealed. Their implications to the ground state symmetry will also be discussed.

Development of Tunable VUV-laser-based *μ*-ARPES System at HiSOR

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ABSTRACT

Angle-resolved photoemission spectroscopy (ARPES) plays an important role for the investigation of the physical properties of solids. Owing to greatly improved energy and momentum resolution of modern ARPES, one can now directly determine not only the energy (ω) and momentum ($\boldsymbol{k}$) distribution of electrons, but also $\boldsymbol{k}$-resolved energy-gaps, and many-body interactions in solids [1]. For high-resolution ARPES experiments using vacuum-ultra-violet (VUV) light source such as synchrotron radiation and He discharge lamps, well-defined clean sample surfaces should be indispensable due to the significantly short mean free path (~10 Å) of photoelectrons [2]. The sample surface for VUV-ARPES experiments can be obtained from *in situ* preparation by cleaving, fracturing, scraping, or sputtering and annealing the sample in ultra-high vacuum. However, the prepared sample surface often possesses micron-order or even larger defects, distortions, and impurities, all of which may lead to the broadening of the spectral features and increase uncertainty of the ARPES data. One of the straightforward ways to overcome this problem is to use the well-focused light. With a spot size smaller than 10 μm, one may have more chance to selectively measure signals from a clean, flat, and homogeneous portion of the sample surface. We have therefore started to construct and develop a tunable VUV-laser-based μ-ARPES system at Hiroshima Synchrotron Radiation Center (HiSOR).

The tunable VUV-laser light source was composed of the commercial mode-locked Ti:sapphire laser and high-order harmonic generator. The generated fourth harmonic is tunable from 191 nm (6.49 eV) to 210 nm (5.90 eV) with high repetition rate (>80 MHz), long pulse width (>10 ps), and high photon flux higher than ~10^{14} photons/sec. By using this tunable VUV-laser, we have experimentally confirmed extremely high energy and momentum resolutions (better than 470 μeV and 0.0048 Å^{-1}). The installation of focusing lens in air is also in progress and the calculated spatial resolution is less than 3 μm. The current status of our VUV-laser-based μ-ARPES system and some representative results will be demonstrated.

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ARPES Study of the Topological Insulator Bi_2Te_3 with a Natural p-n Junction

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ABSTRACT

Topological insulators (TIs) have insulator like bulk whereas on the surface strong spin-orbit coupling produces topologically protected surface states (SSs) with Dirac-type dispersion cone. TIs have exotic electronic properties and high potential to be used in spintronics and quantum electronics. By using the modified Bridgman method, single crystals of Bi2Te3 were grown with the built-in p–n junction formed along the crystal growth axis and perpendicular to the cleavage (0001) plane. In the grown crystals, the p–n junction was observed at all temperatures and its location depended on the initial Bi/Te ratio in the melt [1]. The changes in the Bi/Te ratio during the growth process and, as a consequence, the compensation for the p-type majority carriers are caused by the Te segregation to the top part of the boule. The availability of such material is quite promising since the compensated bulk volume should show no electric conduction. Also, the existence of a lateral p–n junction promises to extend the variety of spintronic applications such as the topological p–n junction and the dual gate TI device. The most common technique used to study TI is angular resolved photoelectron spectroscopy (ARPES). Here we are reporting ARPES studies exploring along natural p–n junction and some peculiar features are identified. As expected, it is possible to fabricate the junction between p-type and n-type topological insulators by composition to achieve spatially variable Dirac cone structures [2]. The electronic structure of the surface p-n junction is different from clean p- and n- type Bi_2Te_3 and also consists of a single Dirac cone. Also we investigated the electronic structure of the clean p-and n-type Bi_2Te_3(0001) surface and its modification upon Cs adsorption using ARPES experiments [3]. We discuss calculated spectral features of Bi_2Te_3, with different level of doping and with corresponding experimental data.

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VUV Laser Angle-resolved Photoemission Spectroscopy Study on the Electronic Structure of the Extraordinary Magnetoresistance Material WTe2

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ABSTRACT

In a unique layered transition-metal dichalcogenide WTe_2, the extremely large and non-saturating magnetoresistance has recently attracted considerable attention [1]. Here, we report a systematic study of its electronic structure by performing VUV-laser based angle-resolved photoemission spectroscopy with super high resolution and statistics. We observed more clear and abundant band structure near Fermi level than that reported by I. Pletikosic et al.[2].There exist two hole-like Fermi pockets and an electron-like one along Gamma-X direction, which has good agreement with our LDA band structure calculation. In particular, at the Brillouin zone center, a quite shallow flat band was found at about 5meV below Fermi energy. The gradual size change of both hole and electron pockets with temperature was observed. Many effects of electron-hole compensation, van Hove singularities and spin-orbital coupling on the unusual large magnetoresistance were discussed.

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Surface States Dimensionality Transition of Bi(111) on a Curved Crystal

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ABSTRACT

Bismuth is a semimetal whose surface shows better metal behaviour than its bulk counterpart due to the presence of metallic-like surface states. These are spin-split given its large atomic weight and spin orbit interaction [1]. Depending on the crystal termination these states behave as two dimensional (2D), delocalized states, or one dimensional (1D), localized states [2]. Such modification of the electron wavefunction is induced by the presence of step arrays, by repulsive scattering at steps and confinement within terraces [3] and has been widely explored for Shockley states in noble metals [3-8]. Semimetals have not received such a widespread attention but the investigating of this 2D to 1D transition is particularly interesting since Bi is very close to being a topological insulator and great interest has emerged in topologically guaranteed 1D surface states.

We present a study that finely explores the 1D-2D transition in Bismuth surface states using a curved crystal (see FSM images). Such special samples allows for a smooth variation of the surface orientation, which translates into a smooth variation of the step separation, i.e. the step potential barriers. The evolution of the electronic structure is investigated by state-of-the-art ARPES and correlated to the local structure obtained from STM and LEED. We find that this transition is very different from the noble metal curved surfaces because we do not observe umklapps and also the surface states are referred to the rhombic (111) direction of the crystal instead of the projection of the *L* point on the surface. Such results, to our knowledge, have never been reported.

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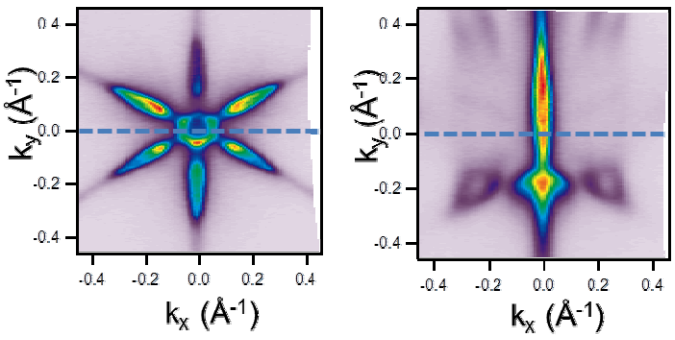

Spin-orbital Texture in the Surface Electronic Structure of Bi-based Rashba Systems

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ABSTRACT

In non-centrosymmetric environments, such as interfaces or surfaces, strong spin-orbit coupling induces large Rashba-type spin splittings in the electronic structure. Among the material systems with the largest known spin splittings are the surface alloy $BiAg_2$/Ag(111) and the polar semiconductor BiTeI. For both materials the splitting and spin texture of the bands are only insufficiently described by a simple Rashba model. In particular, a strong interplay of the spin texture and the orbital composition of the bands has been predicted by theory and experimentally investigated [1,2].

In this contribution we will present spin- and angle-resolved photoemission experiments for the two above-mentioned compounds. Measurements acquired with s- and p-polarized light for surface states of BiTeI indicate a dependence of the spin texture on orbital character. Furthermore, a spin texture inversion between conduction- and valence-band derived states is found. Both observations are in line with theoretical predictions for the ground state spin structure in this material [1,3]. Surprisingly, in the case of $BiAg_2$/Ag(111) the measured spin texture is found to be largely independent of light polarization, in contrast to the predictions of dedicated photoemission calculations [2]. On the other hand, variation of the photon energy is found to substantially modify the photoelectron spin polarization in this system.

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Out-of-equilibrium Electron Dynamics of $ZrTe_5$

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ABSTRACT

Transition-metal pentatellurides, $ZrTe_5$ and $HfTe_5$, have received considerable attention since the 70s owing to their anomalous transport properties (i.e. the peak resistivity at 65 K for $HfTe_5$ and 170 K for $ZrTe_5$ and the change in sign of the hall coefficient and of the thermopower)[1].

Different models, such as charge-density-wave formation, polaron formation, semimetal-semiconductor phase transition[2], have been proposed to explain this anomaly paving the way for an intense discussion about the underlying physics.

We exploit Angle Resolved Photoemission Spectroscopy (ARPES) and time resolved ARPES (tr-ARPES) in order to explore the band structure of $ZrTe_5$ and its evolution at the sub-picosecond time scale.

We reveal the presence of an electron-like unoccupied band at the Γ point, whose dynamic differs from the one of the occupied valence band. We investigate in details the out-of-equilibrium evolution of the band structure, relating it to the peculiar transport properties of the compound.

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Evidence of Inter-band Scattering between Pi and Sigma Bands of Graphene

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ABSTRACT

The electronic structure of graphene has attracted interest over the last few years, hosting several exotic physics phenomena such as quantum Hall effect and Berry's phase [1]. Graphene provides a perfect laboratory for exploring electronic correlations in a two-dimensional (2D) system and their potential for novel applications. In this framework, many body effects play an important role affecting the electronic structure of this material and modifying the behaviour of the electrons in the 2D carbon layer [2, 3]. Despite the vast amount of studies aimed to understand and control many body effects, interactions between pi and sigma bands of graphene have never been experimentally demonstrated because they are usually considered prohibited due to the orthogonality of the orbitals from which these bands derive. Such interactions are reflected in changes in the electronic band structure of a system, in particular the electronic structure line-width is affected.

Combining angle resolved photoemission spectroscopy (ARPES) and density functional theory calculations (DFT) allows to detect and understand the existence of inter-band transitions in graphene, opening up the possibility for exploring new physics phenomena, to contribute for the development of novel electronic devices and hinting at the possibility of engineering a superconducting phase.

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New Opportunities at the APS: The Intermediate Energy X-ray Beamline

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ABSTRACT

The new intermediate-energy x-ray (IEX) beamline at the Advanced Photon Source, Argonne National Laboratory is being developed to investigate collective behavior in interacting electron systems using two distinct but complementary techniques: angle resolved photoemission spectroscopy (ARPES) and resonant soft x-ray scattering (RSXS). This premier facility begins with a state-of-the-art insertion device, the electromagnetic variable polarizing undulator (EM-VPU) with which users can optimize beam properties by the selection of polarization (horizontal, vertical, or circular), and higher-order harmonic suppression via the ability to run in quasiperiodic mode. The optical system is based on an in-focus variable line-spacing plane grating monochromator (VLS-PGM) equipped with three gratings. At 1000 eV the high-flux grating will deliver 10^{12} photons/s with a resolving power of 2500, and the high-resolution grating will deliver 50,000 resolving power and 10^{10} photons/s. Refocusing mirrors focus the beam to a 21 μm × 10 μm (fwhm) spot into an ARPES chamber equipped with a six-axis low-temperature (<10K) goniometer, or a 300 μm x 70 μm spot in the RSXS which features a kappa diffractometer, sample cooling (20 K) and an array of detectors including a photodiode, delay line MPC area detector, and transition edge sensory (TES) energy resolving detector. In this talk the results from ongoing commissioning activities will be presented.

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Influence of the Fermion Density on the Manifestations of Electron-phonon Interaction in ARPES

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ABSTRACT

Comparison of experimental data and theoretical results for optical conductivity [1] and ARPES [2] in high temperature superconductors indicates that the manifestations of electron-phonon coupling, obviously strong in slightly doped compounds, quickly decrease when doping increases. This conclusion was reached by comparison of experimental data at finite carrier densities with theoretical results based on low density limit [1, 2]. Such comparison is doubtful because experiment and theory are compared at different fermion density regimes. Strictly speaking, convincing proof requires accurate treatment of a system with electron-phonon coupling ranging from single polaron to large densities where Fermi energy ε_F is much larger than the phonon frequency ω_0.

Accurate unbiased solution for a problem of polarons at finite densities was missing because numerous avoiding approximations approaches were disabled by famous Fermion sign problem. Recently developed Bold Diagrammatic Monte Carlo (BDMC) technique [3] is capable of giving accurate unbiased results in the range from a single polaron to a dense system, including the most interesting region $\varepsilon_F \approx \omega_0$ where all other numeric and analytic techniques fail.

We start from the single polaron case at strong coupling $\lambda>1$, fix the strength of dimensionless electron-phonon coupling constant λ and study manifestations of the coupling to phonons (effective mass m*, Z-factor of the quasiparticle peak, ARPES) in the range from the single polaron limit to high fermion density regime $\varepsilon_F >> \omega_0$. It is shown that the most drastic changes occur in the nonadiabatic region $\varepsilon_F \approx \omega_0$ where strong manifestations at $\varepsilon_F << \omega_0$ substantially decrease and turn to manifestations imitating weak coupling $\lambda<1$ case at $\varepsilon_F >> \omega_0$. We show that the suppression of manifestations is related to Migdal's theorem which proves that the vertex corrections in Feynman diagrammatic expansion are supressed by the factor ω_0/ε_F.

The main conclusion which follows from our unbiased technique is that the evaluation of the dimensionless electron-phonon coupling constant λ from the high density experiments is a fraud. The manifestations of electron-phonon coupling at large densities imitate $\lambda<1$ coupling strength regardless of the actual strength, $\lambda>1$ or $\lambda<1$, of the electron-phonon interaction. Our data explain doping dependence of the optical conductivity and ARPES in high temperature superconductors.

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Spectral Properties of a Doped Hole in the Hubbard Model

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ABSTRACT

The motion of a single hole in the half-filled two-dimensional single-band Hubbard model is not fully understood, despite the fact that it constitutes a crucial first step in unraveling the doping evolution of the electronic properties of this model system. Here we investigate those hole dynamics, and by extension spectral properties, as well as those of the t-J model and its variants including additional corrections such as the intra-sublattice effective hopping or "3-site" terms,[1] both at half-filling and as a function of hole doping using cluster perturbation theory (CPT).[2] We pay considerable attention to low doping using a "supercluster" construction in CPT to elucidate the initial evolution of the spectrum from the Mott insulator toward the unrenormalized metallic state, which must exist at some large doping value.

At half-filling we find dynamics governed by a complex interplay between (i) the strong coupling of a hole to magnons and (ii) the strongly renormalized, but effectively free, next-nearest neighbor hopping resulting from additional delocalization pathways such as those associated with the 3-site terms. This leads to two distinct features in the spectrum: (1) the "spin polaron" at low binding energies and (2) a main, well separated, dispersive feature at high binding energies. Both features have energy scales equivalent to J; however, the main dispersive feature results almost exclusively from the effective hopping, whereas the "spin polaron" displays a significant influence from both effects, rather than solely coupling to magnons. These claims are further supported by results from the self-consistent Born approximation (SCBA)[3] for the various t-J models. With light hole-doping a third feature forms which disperses across the Fermi level, rapidly stealing spectral weight from the "spin polaron". The doping evolution of this third feature is of particular importance as it constitutes the lowest energy degrees of freedom, those near the Fermi level, in the model. The three spectral features appear distinct, up to a relatively modest doping (~ 12.5%) where the spectral weight effectively has been exhausted in the "spin polaron". We comment on the similarities, differences, and implications for the spectrum in doped cuprates and on competing interpretations of the spectral properties in the Hubbard model, including 2D analogs of complete or partial spin charge separation.[4,5]

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New Electron States at the Bi/InAs(111) Interface

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ABSTRACT

The Bi(111) surface is a prototype system to study Rashba-split surface states. Theoretical studies [1] predicted non-trivial topological surface states appearing on a single bi-layer of Bi(111) and a more complex behaviour was suggested for a variable film thickness as a function of layer thickness [2]. This clearly indicates that the electronic properties of thin films of this material are far from being understood. Here we present combined theoretical and ARPES studies of the electronic structure of Bi(111) films grown on InAs(111).

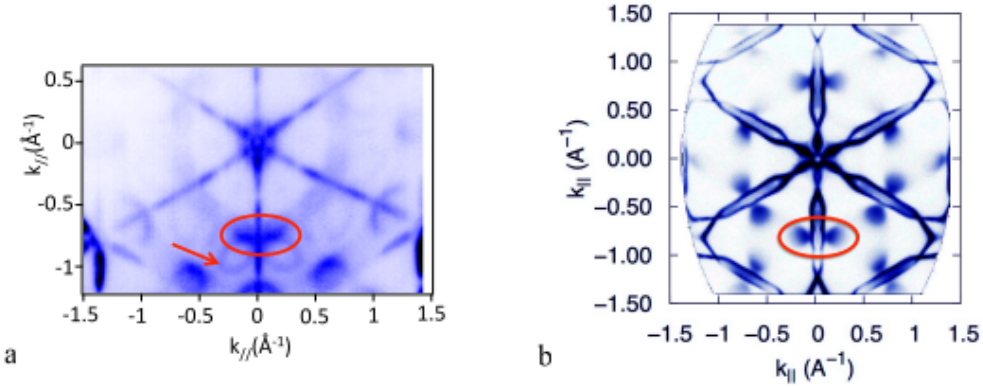

Fig. 1. Fermi surface measured on 10 bi-layers of Bi/InAs(111)(a) and calculated with the help of the SPR-KKR package (b). The new states close to the $\bar{M}$ point are indicated by red lines. The arrow in (a) shows the surface states corresponding to the 6x1 reconstruction. Blue colour means high photoemission intensity.

Bismuth growth is epitaxial and a Bismuth monocrystal of very high quality is obtained after depositing several monolayers. The ARPES experiments on these samples show several new types of electronic states. We show that a proper description of the photoemission process is necessary to understand them. In particular, it is shown that a part of these new states corresponds to novel bulk-like features observed close to the $\bar{M}$ point because a n-doping of the Bi(111) is taking place. These features are well reproduced by the one-step model of photoemission as implemented in the SPR-KKR package [3].

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Two-hole Excitation Spectra of the Extended One-dimensional Hubbard Model

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ABSTRACT

We calculate the two-hole Green's function for the extended one-dimensional Hubbard model using the Chebyshev polynomial expansion technique based on matrix-product states [1]. The related spectral density represents the bare line shape in high-resolution Auger spectroscopy. For an initially filled conduction band this constitutes a two-particle problem which has been solved exactly by Cini and Sawatzky in 1977 [2]. If the Hubbard interaction U is sufficiently strong compared to the free bandwidth W, this solution shows a strong correlation satellite at high binding energies which can be interpreted as a situation where the two holes are repulsively bound [3] and propagate through the lattice as a composite doublon.

When lowering the filling, we observe another resonance which is identified as a three-hole bound state. It has a fine structure and consists of two subpeaks separated by 2t (where t is the hopping) and gains additional spectral weight when increasing the nearest-neighbour Coulomb interaction V. At fillings below n≈1.5, we observe yet another resonance corresponding to a four-hole bound state. Our interpretations rely on the dependence of the peak positions on U and V and are corroborated by an analysis using auxiliary Green's functions with filtered eigenstates. In addition, we compute k-resolved spectral densities to investigate the dispersion of the resonances and to separate broadening effects due to finite lifetime from finite widths due to dispersion.

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The Electronic Structure of Superconducting Cu Intercalated Bi_2Se_3

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ABSTRACT

Recently, superconductivity was found in Cu intercalated Bi_2Se_3 with Tc of about 4K. This caused excitement in the community as it is believed that this system is the first example of a topological superconductor, a superconductor which has non-trivial topological properties.

This discovery led Fu and Berg [1] to provide a sufficient criterion that can be used to identify time reversal invariant 3D topological superconductors (TSCs). A superconductor that has an odd-parity order parameter and that its Fermi-surface encloses an odd number of Time Reversal Invariant Momenta (TRIM) points is a 3D topological superconductor.

Evidence for non-trivial superconductivity in $Cu_xBi_2Se_3$ was provided by point-contact spectroscopy. The spectra have shown Zero Bias Conductance Peaks (ZBCP) [2] which is believed to be a signature of dispersive Majorana modes.

On the other hand, we have recently shown that $Cu_xBi_2Se_3$ [3] does not satisfy the Fu and Berg criterion since the superconducting samples always have open Fermi-surface which encloses two TRIM points. This leaves a few open questions: What is the origin of ZBCPs? Can it be that $Cu_xBi_2Se_3$ is a TSC after all? Can $Cu_xBi_2Se_3$ be a 2D TSC?

We try to answer these questions by performing ARPES experiments on better crystals. Using an electro-chemical intercalation method [2] to prepare $Cu_xBi_2Se_3$ we managed to increase the superconducting volume fraction of our crystals to about 90%. The ARPES spectra of these crystals is very different compared to the spectra of Bi_2Se_3 and from the spectra of previously studied $Cu_xBi_2Se_3$.

We find this kind of spectra only in 1 out of 10 measurements. We suggest that this new spectra represents the superconducting samples and explain why superconductivity in $Cu_xBi_2Se_3$ is so elusive. We also perform ab-initio calculations in order to support our findings, and compare our calculations to other DFT works.

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Self-organisation of Bi on InAs(1 1 1)

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ABSTRACT

Intense experimental research activity is concentrated on thin layers of parent compounds of topological insulators, like Bi, e.g. [1, 2]. It was also predicted by first principles calculations that ultrathin freestanding Bi-films are topological [3]. So far Bi-films were grown on Si [1,2].

In this contribution we present PhotoEmission Electron Microscopy (PEEM) studies on an alternative substrate, the InAs crystal. Thick (30 ML) Bi film deposition on the InAs(111)-A and a subsequent annealing at ≈ 600 K leads to self-organized circular structures with the diameter of several μm (figure 1).

Spatial analysis of Bi *5d*, In *4d* and As *3d* core-level photoemission spectra shows that the circular patterns are composed of unaltered InAs substrate coverd by a thin Bi layer. The spots in the middle of the circles are Bi cristallites and the region in between them are In-poor and As-rich ternary compounds.

From the *k*-resolved PEEM spectra along the $\bar{\Gamma}-\bar{M}$ line we estimate that the medium thickness of the Bi-layer is approximately one monolayer. The InAs(111)-B side shows no particular morphology but stronger chemical shifts of the core-level spectra evidencing Bi-As bonds.

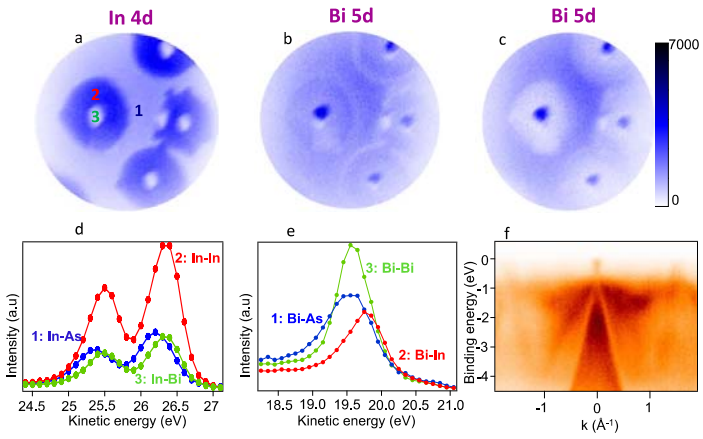

Figure 1.

14 μm diameter PEEM images corresponding to (a) the kinetic energy at the maximum signal of In 4d and to
(b) and (c) two different kinetic energies in the Bi 5d spectrum
In 4d and Bi 5d photoelectron spectra corresponding to the regions 1, 2 and 3 of (a) are shown in (d) and (e).
(f) ARPES spectrum along the $\bar{\Gamma}-\bar{M}$ direction.

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Probing the Geometric and Electronic Structure of the Surface of the Topological Insulator $TlBiSe_2$

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ABSTRACT

After its discovery as a topological insulator with a 3D non-layered structure [1], $TlBiSe_2$ has attracted interest due to the possibility to tune its Dirac point across the Fermi level. The absence of a preferential cleaving plane, like in layered materials, has raised the question of the termination and overall nature of the fractured $TlBiSe_2$ surface and its influence on the formation of the topological surface state.

By combining Scanning Tunneling Microscopy (STM) as well as photoelectron spectroscopy (PES) we were able to identify monolayer high islands covering the fractured surface and the presence of a strong surface core-level shift in the Tl 4f and Tl 5d peaks suggested that half a monolayer of Thallium with a reduced out-of-plane lattice constant was covering a selenium terminated surface [2]. In this presentation we show results from our continued investigation of this surface by means of x-ray and ultraviolet photoelectron diffraction (XPD & UPD) and scanning tunneling spectroscopy (STS) as well as ab-initio theory (DFT) and Angle Resolved Photoelectron Spectroscopy (ARPES) in the UV and Laser photon energy ranges.

We unambiguously answer the question of the island composition and estimate the island-substrate out-of-plane lattice constant, by comparing our XPD and UPD measurements with multiple scattering calculations [3] while taking into account different surface topographies. Based on these structural results, we calculate the band structure and core level spectrum of the $TlBiSe_2$ surface and compare our findings with ARPES and STS measurements. This allows us to explain the emergence of the Tl surface core level shift and shine light on the influence of the island like surface structure on the Dirac Cone.

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Spin and Angle-resolved Photoemission Study of the Surface States on Pb(110)

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ABSTRACT

Recently, spin-polarization of surface-derived states which is originated from a strong spin-orbit coupling (SOC) has attracted much interest since it may have peculiar spin textures and non-trivial topological properties of electron transports at surface [1]. Recently, a Dirac-cone like spin-polarized surface state was discovered on W(110) [2]. This observation suggests that similar surface states may exist in metallic elements with heavy atomic mass.

In this study, we examined the surface electronic states on Pb(110). So far, the bulk-derived electronic states have been studied by angle-resolved photoemission spectroscopy (ARPES) using synchrotron radiation [3]. The observed electronic band structure is reasonably explained by the band-structure calculation with the SOC [3]. However, the surface-derived electronic states are yet to be elucidated.

In this study, we have done polarization-dependent ARPES experiments on the linear undulator beamline at Hiroshima Synchrotron Radiation Center (HiSOR BL-1). Although there is no gap in the bulk band projection, we observed distinct surface-derived states at around the $\bar{\Gamma}$ point of the surface Brillouin zone. These states are not dependent on the incident photon energies, and a band-structure calculation using a slab model could give similar structures. In order to examine the spin-polarization of these states, we have done spin- and angle-resolved photoemission studies using VLEED-type spin detector at HiSOR BL-9B. We found that these surface-derived states are highly spin-polarized and the spin-up and spin-down bands cross at the $\bar{\Gamma}$ point. It confirms that the surface-derived states are spin polarized due to the strong SOC. Our results support that spin-polarized surface-derived states (or surface resonance states) are ubiquitous on the heavy metallic elements.

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Dynamical and Transport Properties of HfB_2, ScB_2 and MgB_2

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ABSTRACT

The phonon spectra, electron-phonon Eliashberg function and T_c of the transition metal diborides were investigated from the first principles using the full potential linear muffin-tin orbital method. The calculations of the dynamic matrix were carried out within the framework of the linear response theory. Comparative analysis of different values T_c, based upon *ab initio* calculation of the electronic band structures as well as the phonon dispersion curves, was performed for row: HfB_2, ScB_2 and MgB_2. Different theoretical approaches (ABINIT, SIESTA, VASP and present LMTO method) to the calculation of the phonon spectra were discussed.

It has been shown that B_{2g} phonon mode in ScB_2 has strong coupling with electronic subsystem and significantly expands middle-energy region on Eliashberg curve. As consequence, averaged electron-phonon interaction constant $\lambda_{e\text{-}ph}$ is reasonably large and equal to 0.47. I obtained T_c =1.62 K (μ^* =0.14) in good agreement with the experimental value 1.5 K. Relatively low value can be explained by smallest ω_{log} among all transition metal diborides. A unique feature of electron-phonon coupling in MgB_2 (T_c=39 K) is the down-shift of the in-plane E_{2g} mode well below the out-of-plane B_{1g} mode (see blue dashed arrow on Fig.) Such inversion of the usual sequence of mode frequencies gives one wide continuous peak formed from medium- and high-energy regions.

On the other hand, HfB_2 out-of-plane B_{1g} mode is shifted down in the vicinity of E_{1u}, A_{2g} modes (see red solid arrow on Fig.). Thus ScB_2 to some extend is situated in the middle between HfB_2 and MgB_2 diborides. Superconductivity in MgB_2 is also related to the existence of B $2p_{x,y}$ band hole along the Γ- A direction. Moreover, the existence of degenerate $p_{x,y}$-states above Fermi level in the Brillouin zone is crucial for the superconductivity in diborides. The 2D $2p_{x,y}$ bands in ScB_2 are partially filled with small hole concentration near A point. On the other hand, the Fermi level for hafnium diboride falls in the pseudogap and the B $2p_{x,y}$ bands are completely filled.

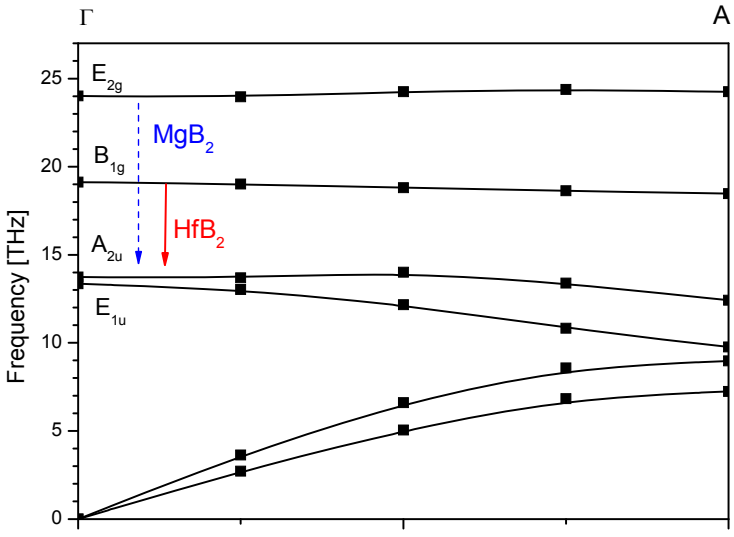

Fig. Theoretically calculated phonon dispersion curves along Γ- A symmetry direction in ScB_2. Dashed blue arrow shows position of E_{2g} mode in case of MgB_2. Red solid arrow demonstrates movement of the B_{2g} phonon mode HfB_2 closer to the E_{1u} and A_{2g} modes.

Momentum Microscopy of Ni-intercalated Layered Semiconductor TiS_2

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ABSTRACT

Atom intercalation into the van der Waals gap of a layered semiconductor TiS_2 can effectively modify its electronic properties in the bulk and surface. In order to probe the changes of its surface electronic structure on Ni intercalation, we have performed high-resolution and simultaneous two-dimensional angle-resolved photoelectron spectroscopy (2D-ARPES) of TiS_2 and $Ni_{1/3}TiS_2$ by use of a momentum microscope and a He lamp. Full (k_x,k_y) band dispersions are revealed up to 2.0 $Å^{-1}$ with the energy resolution of 30 meV for E_B=0 to 5 eV with the step of 25 meV.

Small electron Fermi surfaces (FSs) with noticeable dispersion observed near the M points in TiS_2 became much stronger in $Ni_{1/3}TiS_2$, in which a very small hole FS pocket with clear dispersion is additionally observed near Γ point. The band dispersions near the Fermi level are dramatically changed on Ni intercalation, which also induce noticeable broadening of many dispersive bands. Detailed new experimental results are compared with first principles theoretical band calculations. Differences between these materials are dominated by the contribution of the Ni 3d states of the surface Ni atoms positioned at the C_{3v} site, being different from its D_{3d} site beneath the surface.

The momentum microscopy is demonstrated to be inevitable for clarifying detailed electronic structures of many solids under hot debates, since it can offer almost two orders of magnitude higher counting efficiency than conventional ARPES measurements. In addition, momentum microscopy combined with a 2D-imaging spin-filter offers a concrete basis for high efficiency spin-resolved band-structure measurements, or 2D-SP-ARPES with the efficiency of ~four order of magnitude higher than the single channel spin detection.

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Fermi Surface Analysis of Mott and Charge Ordered Insulator Phases on α-Sn/Ge(111)

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ABSTRACT

Interest on the electronic properties of the α-Sn/Ge(111) interface has been renewed since the discovery of a Mott transition associated to a (√3x√3)R30° symmetry below 30 K[1]. Some doubts were cast on this (√3x√3)R30° Mott phase as the (3x3) symmetry at low temperature was preserved while the metallicity was reduced.

In this work we report a detailed analysis of the valence band electronic structure as a function of temperature by High Resolution Angle Resolved Photoemission Spectroscopy (HR-ARPES)[2]. The analysis of the electronic band structure and the (pseudo)Fermi surface, as a function of the temperature convincingly demonstrate the existence of three different phases below room temperature: a metallic state at 200 K with (3x3) symmetry; a Charge Ordered Insulator (COI) phase at 40 K with (3x3) symmetry and the Mott insulator state at 5 K with (√3x√3)R30°symmetry. These results are in agreement with previous STM measurements[3] and confirm these results as well as the coexistence of the COI phase with the metallic and Mott phases.

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Quantitiative Determination the Fluctuations Responsible for the Superconductivity in Cuprates

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ABSTRACT

I will report on Laser based ARPES of unprecedented accuracy and stability (taken by the group of Xingjiang Zhou, IOP, Beijing), together with a method of analysis (done with the group of Han-Yong Choi, Asia Pacific Center for Theoretical Physics, Korea), to quantitatively extract the many-body effects due the coupling of fermions to the fluctuation spectra in both the full symmetry (normal) and the d-wave sub-group (pairing) symmetry of the lattice in a family of cuprates. The analysis does not depend on any assumption about the mechanism of high temperature superconductivity. We find to an accuracy of about 10% that the attractive electron-electron interaction function, for scattering between momenta k and k' with energy exchanged ω, projected to the d-wave symmetry is the same with a change in sign as that projected to the full symmetry of the lattice. This function is independent of the magnitudes *k; k'*, as well as of ω except at low energies and with a high energy cut-off of about 0.4 eV. The large cut-off together with the logarithmic enhancement to the coupling constants for superconductivity for such a spectra gives rise to the high Tc. Their projection to the full symmetry is repulsive and to the d-wave symmetry is attractive. These results were anticipated in a theory of promotion of superconductivity by quantum-critical fluctuation of loop-currents.

Electronic Band Structure and Spin Polarization Study of WTe_2

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ABSTRACT

WTe_2 is a member of transition metal dichalcogenides. It crystallizes in orthorhombic crystal structure and is subject to structural distortion: the tungsten atoms form chains along the crystallographic a-axis rendering the material effectively one dimensional. WTe_2 is semi-metallic compound, and recently it was found that it exhibits extremely large uniaxial magnetoresistance along the crystallographic c-axis [1], attributed to a balanced electron-hole resonance.

We have measured the electronic band structure of WTe_2 using high resolution ARPES. Our data confirm the existence of small electron and hole pockets along c-direction, as found previously [2]. The comparison with theoretical calculations establishes, however, a significant difference between surface and bulk electronic structure. This finding is further supported by the measurements of shallow core levels. Contrary to W 4f, the Te 4d core level peaks are split in two, indicating two different Te sites, consistent with the theoretical analysis and indicating likely Te surface termination.

We further measured the spin polarization of WTe_2 using spin resolved ARPES and observed a large spin polarization at the hole pocket. This polarization is perpendicular to the W chains (in plane) of the system and changes sign upon crossing the Brillouin zone center (i.e., the two opposite hole pockets have opposite polarization).

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Atomic and Electronic Structures of Homogeneous Quasi-periodic ("2√3×2√3") Silicene on Ag(111)

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ABSTRACT

Silicene, the Si analogue to graphene, has recently been subjected to a large number of experimental and theoretical studies. The calculated electronic band structure is similar to that of graphene which makes silicene highly interesting for applications in Si-based electronics. Theoretical studies of silicene started a few decades ago. Both free-standing silicene and silicene supported by a substrate are predicted to be stable, but only as a slightly buckled sheet[1]. Ag(111) is the most commonly used substrate for the formation silicene. The fingerprint of a graphene like material is a Dirac cone close to the Fermi level formed by a linearly dispersive π-band. An electronic band with a linear dispersion has been reported for silicene in an ARPES study[2] and it was identified as a π-band indicative of a Dirac cone type of band structure. However, this interpretation was recently seriously questioned in a theoretical study[3]. At this point, no electronic band structure has been reported in the literature that can be conclusively assigned to the silicene sheet. The aim of our work was to identify and to characterize electron bands that could be unambiguously assigned to silicene.

We report a detailed and comprehensive study of the atomic and electronic structure of the ("2√3×2√3") silicene on Ag(111) using low energy electron diffraction (LEED), scanning tunneling microscopy (STM) and angle-resolved photoelectron spectroscopy (ARPES). LEED showed a diffraction pattern corresponding to an unconventional rotated ("2√3×2√3") reconstruction. STM images revealed a homogeneous surface with a local (2√3×2√3) periodicity and a quasi-periodic long range order. The ARPES data show three dispersive bands around normal emission. A comparison of these bands with our DFT calculations of the electronic structure of a relaxed (2√3×2√3) model will be presented. We find a good agreement between the experimental bands and the calculated band dispersions of σ-like bands of the buckled (2√3×2√3) reconstructed silicene. The atomic structure of the silicene sheet will also be discussed. The identification of the electron bands for the ("2√3×2√3") silicene opens up for detailed studies of the band structures of other silicene periodicities such as (4×4), (√13×√13), and (√7×√7).

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Direct Measurement of Non-equilibrium Electronic and Phonon Dynamics of $Cu_{0.17}Bi_2Se_3$ via Time Resolved Photoemission Spectroscopy

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ABSTRACT

An application of an extreme ultra-violet laser system to time-resolved core-level and time resolved ARPES enables us to independently determine the time evolution of electron and the phonon temperatures (T_e and T_p) of an electron-doped topological insulator $Cu_{0.17}Bi_2Se_3$. We interpreted ultrafast broadening and recovery of the Bi $5d_{5/2}$ peak in core-level tr-PES as a change of T_p, the scale of which was determined by the temperature dependence in conventional core-level PES. The electronic dynamics and T_e, on the other hand, were determined with near-E_F time resolved ARPES. The extracted dynamics of T_e and T_p did not agree with what were deduced from a simple two-temperature model [1] but did with a modified one [2], implying potential applicability of our method [3].

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The Quantum Materials Spectroscopy Center at the Canadian Light Source

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ABSTRACT

The Quantum Materials Spectroscopy Center (QMSC) currently under construction at the Canadian Light Source (CLS) is a state-of-art beamline facility equipped with endstations for angle-resolved photoemission spectroscopy (ARPES) and spin-resolved ARPES. QMSC will operate in the photon energy range from 10 to 1200 eV, with full polarization control.

The main components of the beamline are the low- and high-energy 4 m long APPLE type undulators, installed side-by-side in a switch-yard arrangement, and a variable line-spacing plane-grating monochromator (VLS PGM). The photon flux will be in the range of 10^{12} – 10^{13} photons/second at the endstations, with a resolving power higher than 10^4 over the full photon energy range. Complete polarization control, in both linear and circular modes, will be available. In addition, the quasiperiodic magnetic structure of the low-energy undulator will guarantee the optimized suppression of higher-order harmonics.

The ARPES endstation is based on a VG Scienta R-4000 hemispherical analyzer with 1 meV energy resolution and a 0.1° angular resolution. The spin-ARPES endstation employs the same analyzer paired with a VG Scienta VLEED single-hole transfer system and spin detector capable of resolving out-of-plane as well as in-plane spin components. The integrated MCP/CCD detector will enable sample alignment and characterization in ARPES mode, prior to spin measurements. A 6-axis cryogenic manipulator installed on both endstations will allow a sample rotation of ±65° and +30° to -70°, respectively, with respect to horizontal and vertical planes. In addition, a closed-cycle cryostat will enable the sample temperature to be quickly varied between 4 and 300K. Both endstations will allow for in-situ sample preparation and manipulation with sputtering, annealing, and adatom evaporation capabilities, as well as the ability to grow oxide materials via integrated molecular beam epitaxy (MBE) systems.

ABSTRACTS

Wednesday, July 8th, 2015

CORPES15

Wednesday, July 8th

Chairpersons: M. Potthoff, T. Tohyama

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K. Haule

IT-TH-15 Matrix product states based impurity solvers for dynamical mean field theory
M. Ganahl

OC-EX-15 ARPES study of the electronic structure evolution in superconducting FeSe
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OC-EX-16 Detailed study of the dramatic reconstruction of the electronic structure of FeSe in the orthorhombic phase
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IT-EX-16 Visualizing electronic structures of topological quantum materials
Y. Chen

OC-TH-17 Theory of Floquet band formation and local pseudospin textures in pump-probe photoemission of graphene
J. Freericks

OC-EX-18 Spin dynamics of hot carriers in the topological insulator Bi_2Se_3
C. Cacho

Hunds Metallicity as the Origin of Anomalous State of Matter in Iron Pnictides and Chalchogenides

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ABSTRACT

The Dynamical Mean Field Theory in combination with the Density Functional Theory has recently enabled detailed modeling of the electronic structure of complex materials, such as heavy fermions, transition metal oxides, chalchogenides and arsenides.

Among those correlated materials, Hund's metals caught a lot of attention recently, because high temperature superconductivity was found in iron pnictides and chalchogenides. Their complex multi-band nature makes the interplay of superconductivity with spin and orbital dynamics very intriguing, leading to very material dependent magnetic excitations, and pairing symmetries. In iron superconductors, the Coulomb interaction among the electrons is not strong enough to localize electrons, but it significantly slows them down, such that low-energy emerging quasiparticles have a substantially enhanced mass, and at intermediate temperature and intermediate energy scale show strong deviations from the Fermi liquid theory.[1] We showed [2] that this enhanced mass emerges not because of the Hubbard interaction U, but because of the Hund's rule interactions J that tends to align electrons with the same spin but different orbital quantum numbers when they find themselves on the same atom. Hundsness [3] rather than Mottness results, which has many similarities but also differences with Mott physics found in many transition metal oxides.

The ab-initio simulations with the Dynamical Mean Field Theory [4] not only uncover the origin of anomalous properties, but also successfully explains the key properties of these material: such as the mass renormalizations and anisotropy of quasiparticles, the crossover into an incoherent regime above a low temperature scale, and the magnetic excitations in energy and momentum space. The ab-initio simulations of the two particle vertex function [5] allows us to study the spin dynamics and superconducting pairing symmetry in a large number of iron-based superconductors. We predicted [6] a novel orbital antiphase s+− symmetry of superconducting pairing, which was not found by either weak coupling nor strong coupling approaches, as it is driven by Hund's coupling in metallic systems. This orbital-antiphase pairing symmetry explains the puzzling variation of the experimentally observed superconducting gaps on all the Fermi surfaces of LiFeAs, and may be realized in other iron superconductors.

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Matrix Product States Based Impurity Solvers for Dynamical Mean Field Theory

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ABSTRACT

The Density Matrix Renormalization Group (DMRG)[1] and Dynamical Mean Field Theory (DMFT)[2] are among the most prominent methods for treating correlated quantum systems. The main obstacle one faces in DMFT is the calculation of the Greens function of an auxiliary impurity system. While Monte Carlo methods are now widely and successfully applied to this problem, they face difficulties when it comes to very low temperatures, calculation of real-frequency quantities and/or non-diagonal baths. I will talk about how Matrix Product States[3,4] techniques and DMRG can be applied as zero temperature and real frequency impurity solvers within DMFT, in particular how real time evolution[5] and the recently implemented Chebyshev[6] expansion techniques can be used to calculate impurity Greens functions[7,8,9,10]. I will present results for the single and two band Hubbard model where we observe sharp features in the density of states also at non-zero frequencies.

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ARPES Study of the Electronic Structure Evolution in Superconducting FeSe.

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ABSTRACT

Among the Fe-based superconductors FeSe with T_c~9K is a special case since it undergoes a structural tetragonal to orthorhombic transition at T_s~87K, but does not order magnetically at any temperature. This material attracted a lot of attention due to the strong increase of T_c up to 37K under high pressure [1] and existence of the high-T_c intercalates [2]. The most intriguing results came from a monolayer of FeSe grown on $SrTiO_3$ where it has been reported increase of superconducting transition temperature up to 100K [3]. Recent NMR study suggests that suppressed orbital-driven nematicity might be a cause for the strongly enhanced T_c in FeSe single layers [4].

In our work we have explored the electronic structure of FeSe single crystals by the synchrotron based high-resolution angle-resolved photoemission spectroscopy (ARPES) with focus on the effects of electron correlations and the evolution of the band structure of FeSe from the high-temperature tetragonal phase to the low temperature orthorhombic phase [5]. The observed dramatic changes in electronic structure cannot be explained by the small lattice distortion effects and, in the absence of the magnetic fluctuations, points towards an electronically driven transition in FeSe with orbital degrees of freedom playing a crucial role.

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Detailed Study of the Dramatic Reconstruction of the Electronic Structure of FeSe in the Orthorhombic Phase

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ABSTRACT

The discovery of iron based superconductors offers new perspectives to understand unconventional superconductivity. In particular, the interplay between superconductivity, magnetism and structural properties is a crucial point that attracts a lot of attention. In these compounds, most of the magnetic phases arise just below a structural transition from tetragonal to orthorhombic. The role and origin of this transition is not well understood. On the other hand, superconductivity usually emerges when the magnetic phase is suppressed through doping or applied pressure, but it may also coexist with magnetism.

The case of FeSe, which is superconducting around 9K, is very interesting since it presents a structural transition at 87K without any magnetic order [1]. As magnetic fluctuations are detected only below the structural transition [1], it suggests that the transition may be stabilized by orbital-charge ordering rather than magnetic fluctuations. The presence and nature of possible nematic fluctuations above the transition are still under debate.

Angle Resolved Photoelectron Spectroscopy (ARPES) allows us to unravel the electronic structure of this compound above and below the structural transition. We observe a large splitting of about 50meV between the dxz and dyz bands in the orthorhombic phase, similarly to other reports [2, 3, 4]. Such changes in the electronic structure largely exceed those expected from the structural distortion of the lattice. We further detail how the number of carriers, the renormalization and the lifetimes evolve through the transition for each orbital. Our data give a precise view on the impact of the orbital order on the electronic structure.

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Visualizing Electronic Structures of Topological Quantum Materials

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ABSTRACT

The discovery of materials with novel properties is one of the most fascinating aspects of physics, and such findings have always played important roles in the development of science and human life. Two recent examples are graphene and topological insulators. Interestingly, both materials possess 2D Dirac fermions; and topological insulators further show distinct topology in their electronic band structures. With the swift development in both fields, two questions have been naturally raised:

i). Does there exist a 3D counterpart of graphene, or a “3D graphene”?
ii). Besides topological insulators, can one find other materials that have unusual topology in their electronic structures?

Remarkably, the answer to both questions can lie on a same type of novel quantum matter – the topological Dirac semi-metal - which not only processes 3D Dirac fermions in the bulk (in contrast to the 2D Dirac fermions in graphene and topological insulators), but also shows unusual topology in its electronic structures.

In this talk, I will show that by using advanced photoemission spectroscopy with high energy, momentum, and time resolution, we were able to directly visualize the non-trivial electronic structures and unusual dynamics in topological insulators and topological Dirac semi-metals recently discovered.

Theory of Floquet Band Formation and Local Pseudospin Textures in Pump-probe Photoemission of Graphene

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ABSTRACT

Ultrafast materials science promises optical control of physical properties of solids. Continuous wave circularly polarized laser driving was predicted to induce a light-matter coupled state with an energy gap and a quantum Hall effect, coined a Floquet topological insulator. Whereas the envisioned Floquet topological insulator requires high frequency pumping to obtain well-separated Floquet bands, a follow-up question regards the creation of Floquet-like states in graphene with realistic low-frequency laser pulses. Here we predict that short optical pulses attainable in experiments can lead to local spectral gaps and novel pseudospin textures in graphene. Pump-probe photoemission spectroscopy can track these states by measuring sizeable energy gaps and Floquet band formation on femtosecond time scales. Analyzing band crossings and pseudospin textures near the Dirac points, we identify new states with optically induced nontrivial changes of sublattice mixing that leads to Berry curvature corrections of electrical transport and magnetization.

Spin Dynamics of Hot Carriers in the Topological Insulator Bi_2Se_3

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ABSTRACT

Topological Insulators (TIs) are attracting widespread scientific interest, particularly for their surface electronic spin structure [1]. The prospect of photoinduced spin polarized currents for spintronic devices requires an in-depth understanding of the out-of-equilibrium electronic dynamics [2]. What are the empty states available above Fermi and how do the hot carriers relax between bulk and surface? Here we report a time- spin- resolved ARPES study [3] on n-doped Bi_2Se_3 in order to explore the electronic relaxation above the Fermi level in both spin channels. The sample is optically pumped with 1.55 eV photon energy and probed with 6.2 eV photon energy for photoemission. The ARPES measurement is performed with a spin-resolved electron Time-of-Flight analyser which allows us to resolve the spin of the photoelectron over several orders of magnitude on the photoemission signal.

Our experiment reveals for the first time the existence of a spin polarized surface resonance state (SRS) in Bi_2Se_3 with a topologically trivial character. These out-of-equilibrium measurements are very well reproduced by fully relativistic ab-initio spin resolved photoemission calculations [4] populated by a hot Fermi-Dirac distribution (Te = 850 K). Furthermore, the study of the energy- and spin- dependent relaxation of the hot carriers allows us to disentangle the bulk and surface electron thermalization. The difference in cooling rates of both systems is attributed to the presence of the SRS acting as a bottleneck in the relaxation process which also results in a weak coupling between the topologically protected surface state and the bulk conduction bands. Our findings may have important implications for the optical control of spin currents in TIs and points towards the possibility of independently manipulating the surface and bulk spin states.

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ABSTRACTS

Thursday, July 9th, 2015

CORPES15

Thursday, July 9th

Chairpersons: S. Molodtsov, A. Taleb-Ibrahimi, M.C. Asensio

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L. Perfetti

IT-EX-18 Electronic and bosonic excitations in high temperature superconductors analyzed by time-resolved ARPES
U. Bovensiepen

OC-TH-19 Probing the atomic scale magnetic structure via spin-flip, orbital-flip and chiral excitations in resonant photoemission
F. Da Pieve

OC-EX-20 Soft-X-ray ARPES investigation of chromium dioxide: More insight into the electronic correlation
F. Bisti

IT-TH-19 Elastic and inelastic scattering in attosecond streaking spectroscopy of solids
E. Krasovkii

IT-TH-20 Explicit role of O 2p states in high oxidation state (transition metal) oxides
G. Sawatsky

IT-EX-21 Low energy excitations in cuprate high temperature superconductors
I. Vishik

IT-TH-22 Excitonic condensation of strongly correlated electrons
J. Kunes

OC-TH-21 Theoretical spectroscopy for correlated materials: Rethinking the interface of electronic structure and many-body theory
S. Biermann

OC-EX-22 Direct observation of momentum-dependent heavy fermionic electronic structure for $CeNi_2Ge_2$
Y. Nakatani

OC-EX-23 Symmetry of the Fermi surface and evolution of the electronic structure across the paramagnetic-helimagnetic transition in MnSi/Si(111)
A. Nicolaou

Dynamics of Electronic States in Correlated Materials and High Temperature Superconductors

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ABSTRACT

I will present time resolved photoelectron spectroscopy data of La_2VS_3 and of high temperature superconductor $Bi_2Sr_2CaCu_2O_{8-x}$.

The misfit compound La_2VS_3 is insulating up to high temperatures although band structure calculations predict a finite density of the electronic states at the chemical potential. The breakdown of the Fermi liquid theory is monitored in the reciprocal space by angle resolved photoelectron spectroscopy. It follows that La_2VS_3 holds a pseudogap which scales as the incommensurate V-V distortion of the VS_2 layers. Upon photoexcitation, the electronic states relax energy in to phonon modes and the pseudogap is partially filled. In contrast to charge density wave compounds, the observed dynamics is faster than 80 fs. We ascribe the sudden melting of the pseudogap to the strong electron-phonon coupling of the aperiodic V-V potential.

New data on $Bi_2Sr_2CaCu_2O_{8-x}$ reveal interesting aspects of photoexcited superconductors. The electrons dynamics show that inelastic scattering by nodal quasiparticles decreases when the temperature is lowered below the critical value of the superconducting phase transition. This drop of electronic dissipation is astonishingly robust and survives to photoexcitation densities much larger than the value sustained by long-range superconductivity. The unconventional behavior of quasiparticle scattering is ascribed to superconducting correlations extending on a length scale comparable to the inelastic mean-free path. Our measurements indicate that strongly driven superconductors enter in a regime without phase coherence but finite pairing amplitude. The latter vanishes near to the critical temperature and has no evident link with the pseudogap observed by Angle Resolved Photoelectron Spectroscopy.

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Electronic and Bosonic Excitations in High Temperature Superconductors Analysed by Time-resolved ARPES

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ABSTRACT

Analysis of excitations in materials is of wide spread interest due to the coupling of electronic and bosonic degrees of freedom, in particular for high temperature superconductors. Typically the spectrum and dispersion of excitations is investigated by e. g. inelastic scattering and angle-resolved photoemission spectroscopy (ARPES). Here we report on femtosecond time-resolved ARPES results on the cuprates and the Fe-pnictides which were obtained by 1.5 eV pump and 6 eV probe photon energies with typically 100 fs time resolution [1]. We discuss how such excitations are probed in tr-ARPES. On the cuprates we have identified a weakening of the well known kink in the electronic structure $E(k)$ at about 70 meV below the Fermi level E_F, which represents a pump-induced reduction of the electron-boson coupling strength [2]. Coupling of electrons to that mode is also evident at an energy of 70 meV above E_F from a step in the energy-dependent electron relaxation times τ(E). A pronounced decrease of the step height in τ (E) with increasing pump fluence reflects that weakening of coupling also above E_F. Experiments on Fe-pnictides exhibit a similar step in the energy dependent electron relaxation times, although the effect is weaker and occurs at higher energies in agreement with e. g. inelastic neutron scattering experiments. Furthermore, electron redistribution upon pump laser excitation modifies the Fermi momentum k_F [2], which allows (a) to transiently change the effective doping level and (b) suggests a new way to probe the dynamic response of the Fermi surface of complex materials.

This work was conducted in collaboration with I. Avigo, S. Freutel, M. Ligges, L. Rettig, M. Sandhofer, J. D. Rameau, P. D. Johnson, P. Zhou, G. D. Gu, H. Eisaki, T. Wolf, P. Gegenwart, H. S. Jeevan, A. F. Kemper, and M. Sentef.

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Probing the Atomic Scale Magnetic Structure via Spin-flip, Orbital-flip and Chiral Excitations in Resonant Photoemission

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ABSTRACT

In many interesting (and non macroscopically magnetic) materials, like topological insulators and non conventional superconductors, determining the spin texture and the local orbital symmetry of valence states is enormously important. While angle resolved photoemission (ARPES) and resonant inelastic X-ray scattering (RIXS) provide relevant information on the angular momentum character of such valence states, their sensitivity to spatial localization is limited due to the linear dependence of the dipole operator to the space coordinate $\underline{r}$. Augmenting the sensitivity to spatial localization is necessarily linked to the fundamental idea of a *localized* valence hole, which remains an elusive notion, and would boost the possibility to perform a full tomography of magnetic degrees of freedom at the atomic scale.

Here I propose that resonant photoemission and related diffraction patterns in the so called participator channel can represent a new way of mapping the both the spin and orbital polarization of valence states with such augmented sensitivity [1,2]. In this emission channel, the decay actually takes place before the hole gets delocalized. Also, as spectral features shows a linear dependence with photon energy, peaks can be distinguished (before and at the very absorption edge) from the Auger-like (spectator) channel, which becomes dominant soon after the edge.

Considering the test case of a simple ferromagnet, here I present ab-initio results on resonant photoemission (at the L_{23} edges) and related diffraction patterns induced by circularly polarized light, calculated via a modified one-step of photoemission in the real space multiple scattering approach, with excitonic effects possibly included via the multichannel “flavor” of such approach [3]. The resulting patterns offer a real space imaging of: a) spin flip-orbital flip excitations, even at energies where spin slip excitations are hidden in conventional energy spectra; b) vortex-like features determined by the rotation of the different ml electronic wave front following the electric field of the light. Both effects are related with the local spin and orbital magnetic structure around the absorber ion. The differences with the partial DOS probed by conventional ARPES, effects related to transition matrix elements and final state effects will be discussed.

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Soft-X-ray ARPES Investigation of Chromium Dioxide: More Insight into the Electronic Correlation

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ABSTRACT

In a group of mostly antiferromagnetic insulating 3d transition-metal oxides, the chromium dioxide (CrO_2) is the only one presenting a ferromagnetic conducting phase. Furthermore, the Fermi surface is composed by the electrons of just the majority-spin polarization, resulting in so-called “half-metallic” behavior. One of the most controversial issues about this material is that its half-metallic property is correctly predicted by simple density functional theory (DFT) calculations based on local spin-density approximation (LSDA). Indeed, it is well known that DFT-LSDA calculations fail the prediction of the electronic structure of most 3d metal oxides. The inclusion of gradient corrections (GGA) gives no improvement for these oxides, that instead is obtained by introducing the on-site Coulomb correlation term, as in the LSDA+U treatment. For the CrO_2, the role of the electron correlation is still under debate with positive or negative supporting arguments depending on the experimental study considered.[1]

In this context the favored experimental technique would be angle-resolved photoemission spectroscopy (ARPES) due to its ability to directly probe the band structure resolved in electron momentum. The main problem is that the CrO_2 surface is metastable at normal condition and, immediately after the synthesis, becomes covered by an amorphous insulating film of antiferromagnetic Cr_2O_3. Therefore, its band structure is not accessible to ARPES technique in the usual, and mostly common, photon-energy range (20-200 eV).

In this talk, we present how the larger probing depth of soft-X-ray ARPES[2] can finally reveal the band structure of the CrO_2. The obtained Fermi surface and band dispersion along main reciprocal space direction have been used as a benchmark for different DFT calculations. We demonstrate that already GGA can appropriately describe the Fermi surface and the dispersion of the valence bands. On the other hand, improvements in the description of the less dispersive (and thus stronger correlated) fully-occupied bands can be obtained with LSDA+U calculations, if the U value is adapted, as fitting parameter, for getting the best agreement. Finally we discuss the improvement obtained by a more realistic treatment of the correlation under the dynamical mean field theory (DMFT).

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Elastic and Inelastic Scattering in Attosecond Streaking Spectroscopy of Solids

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ABSTRACT

The new high intensity light sources have opened wide perspectives in solid state spectroscopy. This talk discusses basic aspects of the laser streaking technique in the attosecond time-resolved photoelectron spectroscopy of solids [1,2] with the focus on the role of photoelectron dynamics.

In the laser-assisted photoemission, an ultra-short pulse of extreme UV radiation creates a photoelectron wave packet with a temporal spread within a fraction of the oscillation period of the laser light. The energy shift of the photoelectron spectrum due to the acceleration by the laser field, as well as the distortion of the line shape, provide information about the temporal structure of the excitation process [1-3].

Here, special emphasis is on the role of the lattice scattering (band structure) of the laser-streaked photoelectron [4]. In the vicinity of band gaps, the strong interaction with the crystal is shown to lead to a distortion and a temporal shift of the streaking spectrogram. Further, the implications of inelastic scattering for the phase shift and the optical potential approach to it are discussed. The classical streaking experiments on W(110) [1,2] are analyzed in terms of conducting properties of the photoelectron final states.

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Explicit Role of O 2p States in High Oxidation State (Transition Metal) Oxides

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ABSTRACT

For late 3d transition metal oxide with formally high oxidation states like Cu3+, Ni3+, Co4+, Fe4+, 5+, Mn 4+, and on a different but it turns out similar note Bi4+, the charge transfer energy for transferring electrons from O to the transition metal may be negative resulting in a formally more correct starting point in which the oxidation state is lowered and holes in the O 2p orbitals are introduced. In this talk we present experimental evidence for this in a number of systems of present day importance and discuss the consequences in terms of magnetic properties and issues such as potential charge disproportionation. We use x ray spectroscopies and model cluster like calculations and variational approaches as well as density functional theory where applicable (SrBiO3) to demonstrate the importance of considering the hole occupation of the O 2p states explicitly and discuss some popular materials like the Cuprates, Nickelates, Cobaltates and SrBiO3 ,from this rather different starting point. I will start with the cuprates and some new exact diagonalization and variational method calculations applicable for the cuprates including also the ARPES spectral function calculations. Here we demonstrate that it is of great importance to explicitly include the O 2p bands resulting in 3 spin polaron like quasiparticle states rather than the conventionally mostly used Zhang Rice singlet single band description. In this relatively new approach we can also explain the "effective" charge disproportionation observed with only very small actual charge motion as well as the charge and magnetic super lattice structure in the insulating rare earth Nickelates. We demonstrate that the low energy scale charge degrees of freedom are mainly of O 2p hole character with very strong electron phonon coupling forming O Octahedra molecular orbital like states in the low temperature phases. I will present arguments that actually these ideas are rather generally applicable to a very wide range of systems of compounds involving high cation oxidation states including systems like Ba(Sr)BiO3 which when doped with K are fairly high temperature superconductors preceding the cuprate era.

Low Energy Excitations in Cuprate High Temperature Superconductors

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ABSTRACT

The phase diagram of the cuprate high temperature superconductors features a number of emergent quantum phases whose microscopic origin is unresolved, and a detailed experimental phenomenology is a crucial starting point for understanding these complex materials. Improvements in sample quality and experiment specificity, including enhancing the capabilities of angle-resolve photoemission spectroscopy (ARPES), have made these sort of comprehensive studies useful and possible. An important development in the ARPES technique is to use a narrow-bandwidth UV laser as a light source, and the superior energy and momentum resolution of laser-ARPES provides unprecedented access to the lowest lying excitations relevant to ground state properties. In the superconducting state of cuprates, the lowest energy excitations are found at the node where the superconducting order parameter is identically zero. We have studied the components of the nodal Fermi velocity both tangential to and perpendicular to the Fermi surface at the node using laser ARPES, and the measured doping dependencies of these quantities challenge earlier data. These results have implications for interpreting low-temperature thermodynamic and transport experiments and for understanding the cuprate phase diagram in terms of low energy excitations.

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Excitonic Condesation of Strongly Correlated Electrons

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ABSTRACT

Competition of several atomic multiplets in materials with strongly correlated electrons, e.g., close to a spin-state transition, may result in an instability leading to a broken-symmetry phase with a long-range order. We have investigated the minimal model exhibiting such behavior, the two-band Hubbard model. Calculation within the dynamical mean-field theory which identify the instabilities of the normal phase [1] as well as results obtained in the ordered phases will presented [2,3]. Besides an Ising high-spin–low-spin order we have observed a phase that can be described as a condensate of spinful excitons. It's order parameter allows several distinct thermodynamic phases. We show that temperature and doping can be used as the control parameters that tune the system between these different phases [3].

We propose that exciton condensation can be found in compounds from the $Pr_{0.5}Ca_{0.5}CoO_3$ family and present static mean-field (LDA+U) calculations, solutions of which exhibit the excitonic condensate. We will analyse these solutions and point out the rich physics arising from orbital degrees of freedom in these systems. The observable consequences of the excitonic order will be discussed.

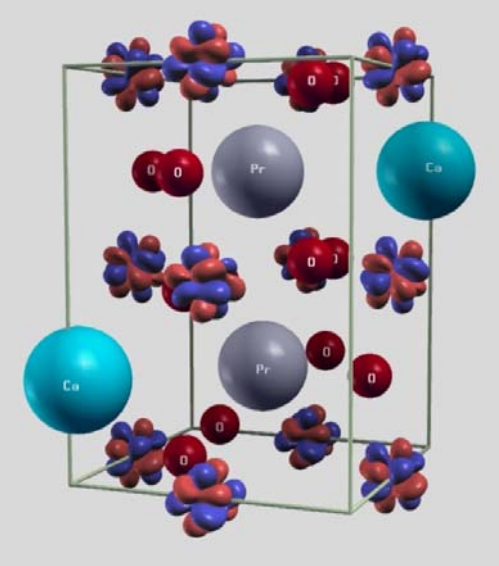

Fig: Spin density around Co atoms in $Pr_{0.5}Ca_{0.5}CoO_3$ induced by exciton condensation.

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Theoretical Spectroscopy for Correlated Materials: Rethinking the Interface of Electronic Structure and Many-body Theory

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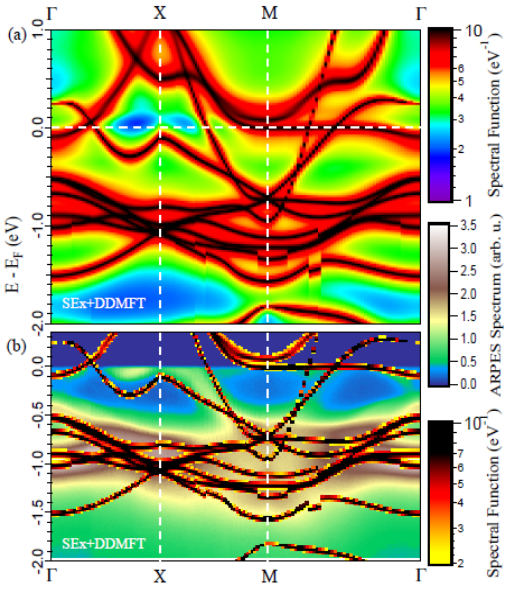
ABSTRACT

Combined density functional (DFT) + dynamical mean field theory (DMFT) has established itself as a method of choice for the theoretical description of spectral properties of correlated electron materials. Nevertheless, increasingly refined applications and attempts to use the theory in a truly predictive manner have also revealed the limits of the current ways of branching many-body theory onto electronic structure calculations [1]. The most subtle points are related to

1. the determination of the effective local Hubbard interactions
2. the dynamical character of these interactions
3. the use of DFT for the one-body part of the Hamiltonian
4. the elimination of double counting issues

Here, we present recent work attempting to push these frontiers forward, by explicitly taking into account dynamically screened Hubbard interactions and a one-body Hamiltonian beyond DFT.

The new “screened exchange dynamical mean field theory” is successfully tested on the transition metal pnictide BaCo2As2 [2] and the ternary oxide SrVO3 [3].



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Direct Observation of Momentum-dependent Heavy Fermionic Electronic Structure for $CeNi_2Ge_2$

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ABSTRACT

The heavy fermion behavior of strongly correlated 4*f* compounds – such as an enormous effective mass enhancement and a superconducting phase transition – has attracted much interest in the field of condensed matter physics. In order to clarify the origin of various physical properties of heavy fermion compounds, the understanding of the formation process of heavy fermionic electronic structure due to *c-f* hybridization is required. However, few studies have focused on the direct observation of heavy fermionic nature due to *c-f* hybridization. We have observed the heavy fermionic electronic structure for the superconducting [1] $CeNi_2Ge_2$. Its electronic specific heat coefficient value is 350 mJ / mol K^2 [2], which indicates the enormous effective mass enhancement due to the effects of *c-f* hybridization. In order to truly probe the heavy fermionic state in $CeNi_2Ge_2$, where the heavy band slope becomes flat in the vicinity of the Fermi level, we have performed soft X-ray angle-resolved photoemission spectroscopy for single crystals of $LaNi_2Ge_2$ and $CeNi_2Ge_2$ at SPring-8 BL23SU. The total energy resolution was ~70 meV at the excitation photon energy of ~700 eV.

Here we provide the unprecedented evidence for the momentum-dependent heavy fermionic electronic structure. An electron-like Ni 3*d* band corresponding to the band 20 in the RLAPW band calculation [3] is observed around the X point, crossing the Fermi level to form a quasi-two-dimensional Fermi surface. This band for $CeNi_2Ge_2$ along the Γ-X direction becomes flat towards the Fermi level to make the Fermi surface larger compared with that for $LaNi_2Ge_2$, being responsible for the heavy fermionic nature. The effective mass of $CeNi_2Ge_2$ along this direction is more than 10 times larger than that of $LaNi_2Ge_2$. This heavy fermion state is absent along the Z-X direction. RLAPW band calculation [3] suggests that the Fermi surface centered at X point formed by band 20 expands for Γ and Z points. However, we find that this Fermi surface expands for only Γ point, which indicates the strength of *c-f* hybridization clearly depends on the momentum. Our finding should also be widely observed for other heavy fermion compounds.

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Symmetry of the Fermi Surface and Evolution of the Electronic Structure across the Paramagnetic-helimagnetic Transition in MnSi/Si(111)

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ABSTRACT

Transition-metal monosilicides, such as TM-Si (TM = Mn, Fe, Co) and their solid solutions, show an intriguing evolution of the electronic and magnetic properties as a function of temperature and doping, including non-Fermi liquid behavior and novel spin structures such as skyrmion phases [1-3]. The weakly itinerant ferromagnet MnSi represents a paradigmatic case for its magnetic properties not accounted for by standard models of magnetism. The value of the saturated magnetic moment in the ordered helimagnetic phase is significantly smaller than the value predicted by the local density approximation (LDA) [4]. Furthermore, the magnetic transition can be progressively suppressed by applying a relatively low hydrostatic pressure p_c = 14.6 kbar, where the system reaches a quantum critical point and enters in a non-Fermi liquid phase characterized by a $T^{3/2}$ dependence of the resistivity and accompanied by a partial magnetic order.

We will present the first experimental determination of the Fermi surface (FS) symmetry and the evolution of the electronic structure across the paramagnetic-helimagnetic transition at T_C□40K by angle-resolved photoemission (ARPES) spectroscopy performed on high-quality MnSi/Si(111) films. The experimental FS, not reproduced by LDA calculations, is found to favor the nesting between electrons and holes, which can be at the origin of strong magnetic fluctuations, not accounted for by the state-of-art many-body calculations in the quasiparticle self-consistent GW approximation. From this perspective, the unusual d-bands broadening observed in the paramagnetic phase, along with the sharp quasi-particle emission we detect at □5K, and the persistence of the d-bands splitting well above T_C, point to a substantial presence of magnetic correlations affecting the quasiparticles lifetime.

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POSTER SESSION II

Thursday, July 9th, 2015

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PO-II-EX-02	Discovery of a two-dimensional liquid of Fröhlich polarons at the bare SrTiO3 surface *M.C. Asensio*
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PO-II-TH-13	Two distinct pseudogaps and quasiparticle tunneling in cuprate superconductors: Evidence for multiple energy gaps on the tunneling spectra *O.K. Ganiev*
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PO-II-EX-15 On the nature of electron localization in the high pressure phase of $LuFe_2O_4$
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PO-II-EX-16 Fermi surface mapping and pseudo-gap of quasi-one-dimensional $Tl_2Mo_6Se_6$
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PO-II-EX-17 Angle-resolved photoemission spectroscopy of correlated electron pairs in NiO And CoO
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PO-II-TH-18 Possible mechanisms of carrier localization, metal-insulator transitions and stripe formation in inhomogeneous hole-doped cuprates.
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T. Kim

PO-II-EX-20 A quantum confined gas of large polarons at the $SrTiO_3$ (001) surface
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PO-II-EX-21 Charge-density-wave transition in LaAgSb2 investigated by angle-resolved photoemission spectroscopy
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PO-II-EX-22 Angle-resolved photoemission study of a thermoelectric and multiferroic delafossite $CuCrO_2$
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PO-II-EX-23 ARPES study of electronic properties of in-situ grown ultra thin $NdNiO_3$ films in proximity to a magnetic underlayer
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PO-II-EX-24 Large energy-scale ARPES spectral modulation with temperature in a layered manganite
T. Saitoh

PO-II-EX-25 Significant doping effect in the annealing process and true phase diagram of electron doped cuprate
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PO-II-EX-26 Momentum dependence of a Kondo resonance in $Ce_2Co_{0.8}Si_{3.2}$
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PO-II-EX-27 Polaronic Effects in 3D systems and buried heterostructures explored by soft-X-ray ARPES
V.N. Strocov

PO-II-EX-28 Soft X-ray ARPES study of the new diluted magnetic semiconductor $Ba_{1-x}K_x(Zn_1\text{-}_yMn_y)_2As_2$
H. Suzuki

PO-II-TH-29 Electronic entanglement and classical correlation in SmB_6
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PO-II-EX-30 Double photoemission spectroscopy on silver and 3d transition metal oxides
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PO-II-EX-31 Laterally anisotropic quantum well states at the surface of anatase TiO_2 (001) thin film unveiled by angle resolved photoemission
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PO-II-EX-33 Bond stretching phonon softening and kinks in the angle-resolved photoemission spectra of under doped $La_{2-x}Ba_xCuO_{4+\delta}$ superconductors
Z. Zhang

PO-II-EX-34 High-resolution angle-resolved photoemission study of Fe/MgO(100)
M. Zheng

PO-II-EX-35 The spectral function of honeycomb Na_2IrO_3 by ARPES upon Li and Ru substitution
M. Zonno

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B. Zwartsenberg

Layer-resolved Resonant Auger Spectroscopy to Probe the Nature of a Metal-supported Ultrathin Oxide Film

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ABSTRACT

On the nanoscale, materials often reveal new and unexpected features. In particular, ultrathin oxide films grown on metal substrate constitute a class of new materials whose interesting and novel properties have raised several questions on the direct and indirect role played by the substrate and reiterate the interrogations concerning the nature of interactions at the metal/oxide interfaces.

By combining x-ray excited Auger electron diffraction experiments and multiple scattering calculations we reveal a layer-resolved energy shift of the Mg $KL_{23}L_{23}$ Auger transition in MgO ultrathin films grown on Ag(001) [1]. We then study the evolution of the layer-resolved Mg $KL_{23}L_{23}$ Auger transition in a photon energy range corresponding to the Mg K-edge. In good agreement with density functional theory (DFT) calculations, we show that the intensity evolution of the resonant Auger spectra with the photon energy allows to get a layer-by-layer mapping of the local density of empty Mg p-states probed by the excited photoelectron in the intermediate dipole transition.

In the pre-edge region, we find that the Auger spectra mostly consist of a single Auger component, the one of the metal/oxide interface, demonstrating the metallic character of the oxide interface layer due to the presence of metal-induced gap states (MIGS). We measure the MgO surface band gap and a spectroscopic fingerprint of a surface core exciton involving an image potential state of the vacuum. Our results demonstrate how to obtain new insights on empty states at interfaces of metal-supported ultrathin oxide films [2].

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Discovery of a Two-dimensional Liquid of Fröhlich Polarons at the Bare SrTiO3 Surface

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ABSTRACT

The polaron, is a quasiparticle formed by a conduction electron (or hole) together with its self-induced polarisation in a polar semiconductor or an ionic crystal[1-5]. Among various polarisable examples, strontium titanate ($SrTiO_3$) is one of the most studied complex oxides, presenting a wide spectrum of phenomena. Recent research has revealed the critical rôle played by its bosonic modes in the strengthening of Cooper pairing in monolayer FeSe. We go a step further to examine the carriers type and the interplay of inner degrees of freedom (e.g. charge, lattice, orbital) in $SrTiO_3$. We report the discovery of the Fröhlich polarons, o large polarons, at the bare SrTiO3 surface prepared by vacuum annealing. Systematic analyses of angle-resolved photoemission spectroscopy (ARPES) and X-ray absorption spectra (XAS) show that these Fröhlich polarons are two-dimensional (2D) and only exist with inversion symmetry breaking by 2D oxygen vacancies. Our discovery provides a rare solvable field theoretical model, and suggests relevance of large (bi) polaron for superconductivity in perovskite oxides as well as in high-temperature superconductors.

In this presentation, by examining the surface electronic structure of vacuum-annealed $SrTiO_3$, we report the discovery of 2D liquid of Fröhlich polaron, a new quasiparticle formed by conduction band electron coupled with one polar longitudinal optical (LO) phonon mode. By controlling the annealing temperature, we can precisely tune the surface oxygen vacancy concentration, which evolutes from a 2D to three-dimensional (3D) distribution of charges. Moreover, by compiling partial electron yield and total fluorescence yield XAS; we have been able to identify unambiguously these two distinctive distributions of oxygen vacancies. In the 2D case, oxygen defect dipoles break the inversion symmetry and initiate the coupling between electrons and polar longitudinal optical (LO) phonons. This intermediate coupling leads to the formation of a new type of quasiparticles, Fröhlich polarons, whose spectra function contains multiple replicas of original bands, equally spaced ω_{LO} apart, with ω_{LO} the effective energy of LO-phonons, as directly observed by ARPES here. Photon-energy dependent ARPES measurements reveal the 2D nature of Fröhlich polarons. In the 3D oxygen vacancy case, the 2D polarons collapse into 3D electron liquid due to the reversal of symmetry. Our finding consist with the effective branch approximation, suggesting stable bipolarons in $SrTiO_3$, and reveal the essential role of LO-phonons-related large (bi) polarons in understanding superconductivity in perovskite oxides as well as in high-temperature superconductors.

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Antiferromagnetic Order and Spin Density Wave in Bulk Chromium Explored by Soft-X-ray ARPES

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ABSTRACT

Chromium metal presents a complex and interesting magnetic structure featuring, at room temperature, an antiferromagnetic (AF) order modulated by a spin-density wave (SDW). In particular, under the Néel temperature of 311 K, there is a transition from the paramagnetic (BCC lattice) to antiferromagnetic (AF) order (SC lattice of CsCl type) modulated by incommensurate (period of ~21 unit cells) SDW along the <100> directions. It is generally accepted that this AF order is induced by Fermi surface (FS) nesting, which connects electron and hole pockets around the Γ and H points of the Brillouin zone, respectively. It is not clear however why the SDW do not stabilize in Mo and W having similar contours of their FS. In view of pronounced three-dimensionality of chromium, ARPES investigations of its electronic structure will benefit from moving into the soft-X-ray energy range bringing sharp definition of the surface-perpendicular electron momentum.

In this talk, soft-X-ray ARPES data on Cr(100) surface will be reported. Investigation on the FS contours, in surface-parallel and perpendicular planes, has allowed to identify the nesting conditions, as well as to distinguish spurious spectral structures related to final-state effects and surface states. Magnetic order has been clearly identified in the electronic structure by the comparison with density functional theory calculations in the presence or absence of AF order. The corresponding spectral replicas demonstrate different spectral weigh depending on the band character.

Massless Gapped Dirac Cones and Many-body Instabilities in Doped Graphene

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ABSTRACT

The low-energy electronic structure of ideal graphene is characterized by a linear cone-like Dirac dispersion with finite band velocity. At the Dirac point the upper and lower cone bands touch each other, making of graphene a zero-gap semiconductor. For technological applications, however, a tunable opening of bandgap is however desirable. Bandgap opening has been previously reported in graphene by using angle-resolved photoemission spectroscopy (ARPES) [1-8] and discussed so far within the framework of a massive Dirac model, where a breaking of the sublattice symmetry gives rise to a massive parabolic behavior at low energies close to the Dirac point. In this contribution we show how recent ARPES measurements of Ir- and Na-modified graphene on Ir(111) surfaces provide a direct evidence of a different (*massless*) scenario [8,9], where the opening of the gap is not accompanied by the onset of a Dirac mass, rather by a splitting of the Dirac linear bands preserving a cone structure [9,10]. We discuss the possibilities and the conditions of establishing such anomalous gap as a result of a spontaneous symmetry breaking [9]. The understanding and possible controlling of this new kind of unconventional gap can open new perspectives in the bandgap engineering of graphene-based materials.

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Electronic Band Structure and Fermi Surface of $Sr_4Ru_3O_{10}$

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ABSTRACT

Ruthenium oxides of the Ruddlesden-Popper series $Sr_{n+1}Ru_nO_{3n+1}$ are particularly attractive materials in the realm of transition metal oxides due to the fact that the interplay between dimensionality, structural distortions, orbital polarization and crystal field splitting results in changes in the competing energy scales which give rise to distinctive collective phenomena ranging from spin-triplet chiral superconductivity to anisotropic magnetic ordering with possibilities of quantum critical behavior [1,2,3]. $Sr_4Ru_3O_{10}$ is the trilayered member of the series, the least studied member of the series, and very little is known about the low-energy electronic structure and its link to the in-plane double metamagnetism [4].

Here we report on the first angle resolved photoemission spectroscopy (ARPES) measurements on the trilayered $Sr_4Ru_3O_{10}$. The data were collected at 5 K at the ARPES end station of the beamline CASSIOPÉE of the synchrotron facility Soleil (Paris, France). We found that the experimental Fermi surface (FS) is constituted by six distinguishable FS sheets. The shape of the FS is compatible with a reconstruction originating from a trilayer splitting and the back folding of bands (due to the 45° in-plane rotation and enlargement of the first Brillouin zone caused by the rotation of the RuO_6 octahedra), of the FS of the single-layered Sr_2RuO_4. The FS sheet(s) derived from the d_{xy} bands in this simple model are however not clearly visible in our spectra.

Furthermore, the line-width of the sharpest low-energy dispersing features is on average quite broad (~20 meV), and roughly twice as much as the energy resolution. This is likely to be an indication of the fact that multiple features are superimposed in the line-shape and could not be resolved with the exploited photon energies and polarizations. Further investigations will be needed in this respect. Two flat bands, belonging to two different FS sheets, were detected, and are shown to give rise to peaks in the density of states located a few meV below the Fermi energy. Finally, the data reveal the presence of kinks in the near-Fermi-level band dispersion, with energies that are in good correspondence with the energy of the phononic modes reported in the literature [5].

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Valence-fluctuations and Peierls Metal-insulator Transition in a Correlated Ferromagnet

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ABSTRACT

$K_2Cr_8O_{16}$, with a Hollandite-structure consisting of chains and tunnels made of CrO_6 octahedra, was recently discovered to show the unique behaviour of ferromagnetism (below T_c = 180 K) followed by a quasi 1-dimensional ferro-metal to ferro-insulator transition (below T_{MI} = 95 K)[1]. Its complex properties are debated in terms of : (i) charge ordering, [2] (ii) Peierls transition in the quasi 1-d chains, [3] or (iii) a strong-correlation induced Mott-Peierls transition [4]. We study the electronic structure changes across T_c and T_{MI}, using a combination of angle-integrated laser photoemission, soft and hard x-ray photoemission, as well as ab-initio band-structure (GGA+U) calculations. From precise measurements, we observe clear temperature(T)-dependent valence fluctuations of Cr^{3+} and Cr^{4+} states across the ferromagnetic transition(T_c = 180 K). The valence fluctuations get locked in the low temperature phase below T_{MI} = 95 K, indicating a novel insulating ferromagnetic phase.

The resonant photoemission results provide an experimental estimate of the on-site Coulomb correlation energy, U. GGA+U calculations show that the ferro-metal to ferro-insulator transition is driven by the presence of both, strong correlations and a structural distortion. Laser photoemission shows that the T-dependent gap, G(T), follows a Bardeen-Cooper-Schrieffer type second-order behavior with a low energy scale gap (2G(0) ~ 35 meV ~ 3.5 k_BT_{MI}), indicating that the metal-insulator transition is not a Mott-Peierls transition, but a genuine Peierls transition. Our study, thus, identifies and separates out the role of strong correlations, structural distortions and valence fluctuations in realizing the ferro-metal to ferro-insulator transition observed in $K_2Cr_8O_{16}$.

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Inelastic X-ray Scattering for Phonon Modes in Hafnium Nitride

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ABSTRACT

With the aim of understanding interactions between electrons and the lattice dynamics of hafnium nitride (HfN) inelastic x-ray scattering (IXS) has been performed on HfN thin films. From first principle calculations and inelastic neutron scattering experiments HfN's phonon dispersion consist of a large gap between acoustic and optical phonon modes [1]. The gap is large enough such that dominate pathways in which optical phonons decay to acoustic modes do not exist potentially leading to long optical phonon lifetimes. An application which can exploit this property of a large gap in the phonon dispersion is the utilization in photovoltaic devices. In conventional photovoltaic devices up to a third of the incident power is lost as heat to the environment due to the thermalization of above bandgap carriers. Thermalization processes of electrons involve emission of optical phonons which subsequently decay into acoustic phonons. However given long enough optical phonon lifetimes and high enough coupling between electrons and optical phonons, electrons may reabsorb optical phonons thus reducing the rate at which thermalization occurs. By exploiting phonon properties of materials with the ability to reduce thermalization losses a photovoltaic device known as the Hot Carrier solar cell [2] is envisaged to be able to achieve high power conversion efficiencies.

Phonon modes at high symmetry points in its Brillouin zone were measured at room temperature. We present the results from IXS measurements taken at the synchrotron beamline BL35XU at Spring-8 [3]. HfN thin films were prepared by sputtering on MgO substrates. Observed acoustic modes and its relative intensities are in good agreement with predicted peaks from modelling.

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What Sets the T_c? Competition between Pairing and Pair-Breaking Interactions in Cuprate Superconductors

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ABSTRACT

In all conventional superconductors the pairing strength alone sets the majority of the physical properties including the superconducting transition temperature T_C. In the cuprate high temperature superconductors, no such link has yet been found between the pairing interactions and T_C. Using a new variant of photoelectron spectroscopy termed the TDoS (Tomographic Density of States) method (1-3) we measure both the pair-forming (Δ) and a self energy/pair-breaking term (Γ_S) as a function of sample type and sample temperature, and we make the measurements over a wide range of doping and temperatures within and outside of the pseudogap/competing order regimes. In all cases we find that T_C is approximately set by a crossover between the pair-forming strength Δ and 3 times the self-energy term Γ_s. In addition to departing from conventional superconductivity in which the pairing alone sets T_C, these results indicate the great importance of the near-nodal self-energy effects, which may be more significant than the competing order/pseudogap effects. Finding a way to control these self-energy/pair-breaking interactions is thus a possible new route towards even higher superconducting transition temperatures.

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Interplay between Superconductivity and Correlations in Low Dimensional Nanostructures

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ABSTRACT

It is known that the electronic states of isotropic superconductors are prohibited inside some characteristic energy window Δ meV around the Fermi surface because of electron pairing. Similar property has been recently observed in various nanoscopic objects (e.g. molecules, nanowires, carbon nanotubes, self-assembled quantum dots) due to the proximity effect, where the penetrating Cooper pairs convert them into superconducting nanoislands.

The proximized nanoobjects often reveal formation of the additional in-gap (subgap) bound states. These Andreev-Yu-Shiba-Rusinov quasiparticles appear always in pairs because they represent coherent superpositions of the particle and hole states. Under specific conditions (due to spin-orbit coupling and external magnetic field) some of the in-gap states may evolve into the Majorana-type quasiparticles. In fact, the first experimental signature of the zero-energy Majorana feature has been reported by the Dutch group from Delft using InSb wire deposited on the s-wave NbTiN superconductor [1].

I shall give a survey on the recent intensive studies of the Andreev/Majorana quasiparticles in nanoscopic systems. I will also discuss some closely related studies on the Cooper pair splitters, where the released/depaired electrons preserve their quantum entanglement over macroscopic scales.

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Analysis of the Band Dispersions of the Bilayer Ruthenate $Sr_3Ru_2O_7$ around the High Symmetry Points

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ABSTRACT

We have investigated the formation of heavy *d* electron quasiparticles in the bilayer ruthenate $Sr_3Ru_2O_7$ by analysing the dispersion of the bands in the proximity of the Fermi level around the high symmetry points Γ and X of the first Brillouin zone. This was done by means of angle resolved photoemission spectroscopy (ARPES) measurements performed at 2 K at the 1^3 end-station at BESSY II. We report the existence of flat bands giving rise to van Hove singularities (vHS) in the DOS a few meV from the Fermi level. These are associated with the γ_2 Fermi surface (FS) sheet centred at the X point with d_{xy} orbital character, and with the α_2 and δ FS sheets centred at the Γ point with hybrid $d_{xz,yz}$ and d_{x2-y2} orbital characters, respectively. These findings are in substantial agreement with previous ARPES results reported on the same system [1,2]. These vHS are deemed to be responsible for the appearance of the multiple metamagnetism observed in $Sr_3Ru_2O_7$, as predicted by Binz *et al.* [3]. In addition, our results show signatures of strong correlation effects, characterized by the peak-dip-hump line shape of the low-energy states, which is generally seen in the band dispersions of strongly correlated electron systems [2]. Finally, we have noted the presence of bands not predicted by electronic structure calculations, which might be band replicas due to the reconstruction of the sample surface.

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Excitation-energy Dependence of Low-energy Excitations in Insulating and Underdoped $La_{(2-x)}Sr_xCuO_4$

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ABSTRACT

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 the O K-edge in the paradigmatic cuprate material $La_{(2-x)}Sr_xCuO_4$ (LSCO), as a function of doping ranging from an insulator to a bad metal (superconductor). Namely, we have studied the doping dependence of a feature at ~ 2 eV energy loss, representing the characteristic Zhang-Rice singlet state [2-3].

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Oxidation of TiN(TaN) by Contact with γ- Al_2O_3

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ABSTRACT

Analysis of different metal-insulator-metal (MIM) and metal-insulator-semiconductor (MIS) structures reveals that the interface between gate dielectric and metal electrode critically determines the effective work function. The mechanisms determining the height of the energy barrier for electrons at metal/insulator interfaces, which direct impact on the functionality of the devices, are of a special interest and under debate up to now. It was demonstrated that in some systems the electrostatic potential at the interface is perturbed by a polarization layer. The interface polarization layer can be modified by carefully depositing both dielectric and metal gate materials followed by a high temperature treatment.

In the current work we are focusing on the study of electrode/Al_2O_3 interface depending on the electrode material, to evaluate the possible oxygen scavenging from the Al_2O_3 insulator. The pre-crystallized Al_2O_3 thin films with top unannealed and annealed electrodes are in the focus of this work. TiN and TaN were chosen as commonly used metal gate electrodes with mid work function. All the studies were performed using Hard X-Ray Photoelectron Spectroscopy (HXPES) and near-edge-x-ray absorption fine structure (NEXAFS) at the Berlin Synchrotron Radiation facility BESSY-II of the HZB. The HXPES and NEXAFS experiments were performed using the HIKE station at the KMC-1 beamline and Polarimeter station at the UE56-2_PGM-2 beamline, respectively.

It was established that thick Al_2O_3 layers in contact with metal electrode provokes the oxygen scavenging into electrode. In the TiN/Al_2O_3 stacks the oxygen scavenging from the Al_2O_3 leads to formation of unbonded nitrogen dissolved in the matrix. Study of the polarization dependence (using the linear and elliptical polarization for the photon) of the OK-absorption spectra points to the occurrence of spin polarization states of the conduction band associated with the splitting of atomic orbitals with distortion of the polyhedron titanium. Another oxidation process was established in the TaN/Al_2O_3 stacks. The oxygen scavenging from the Al_2O_3 in this stack leads to formation of separated phases TaN_x and TaO_x. In contrast to the TiN/Al_2O_3 stacks only slightly noticeable formation of free nitrogen is traced in TiN electrode. The annealing of the electrodes (TiN and TaN) strengthens the observed processes. Should be noted that analysis of the OK-absorption spectra of studied stacks points to formation of F^+ centers (an oxygen vacancy, which has trap a single electron) in the films under both TiN and TaN electrode. The established polarization dependence of the pre-edge region of OK-absorption spectra allows concluding the various reasons of their occurrence.

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Two Distinct Pseudogaps and Quasiparticle Tunneling in Cuprate Superconductors: Evidence for Multiple Energy Gaps on the Tunneling Spectra

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ABSTRACT

Scanning tunneling microscopy and spectroscopy [1–3] and angle-resolved photoemission spectroscopy [4,5] have made significant progress in studying the electronic properties of high temperature cuprate superconductors.

The tunneling spectra of cuprate superconductors exhibit pseudogap (PG)-like features [2,6,7] and gap-inhomogeneity-induced features [2,3,8-10].

We investigate the pseudogap state in high-T_c cuprates and propose specific (simple and generalized multiple-gap) models of quasiparticle tunneling across the high-T_c cuprate superconductor-insulator-normal metal (SIN) junction based on the different mechanisms for tunneling of electrons at positive bias voltage (V>0) and dissociating polaronic Cooper pairs and large polarons at negative bias voltage (V<0), and the gap inhomogeneity (i.e., multiple-gap) picture. We show that the energy scales of the binding energies of large polarons and polaronic Cooper pairs are identified by two pseudogap (PG) crossover temperatures on the cuprate phase diagram. We study the distinctive features of quasiparticle tunneling across the SIN junction by considering the BCS-type density of states (DOS) at V>0 and the combined BCS-type DOS and quasi-free state DOS (originating from the polaron dissociation) at V<0 and the distribution of BCS-like and polaronic gap amplitudes in inhomogeneous high-T_c cuprates. It is shown that most of the unusual features of tunneling spectra such as nearly U- and V-shaped subgap features, peak-dip-hump structure (appearing systematically at V<0) and asymmetry of the conductance peaks and their temperature and doping dependences, and shoulder-like features inside the main conductance peaks can arise in the specific models of SIN tunneling. The experimental SIN tunneling spectra of $Ba_2Sr_2CaCu_2O_{8+\delta}$ are adequately reproduced using these models. Effects of polaronic PG and gap inhomogeneity play a crucial role in determining the shapes of the tunneling characteristics of cuprate superconductors. The relationship between the BCS tunneling gap and SC order parameter in unconventional cuprate superconductors is discussed.

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Short- and Long-living Excited States in Resonant XPS Spectra of *d-f* Element Compounds

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ABSTRACT

The interplay of *d*- and *f*-elements and its effect on the formation of the electronic structure in such compounds as $GdNi_{5-x}Cu_x$, $DyNi_2Mn_x$[1] and (La0PrCa0)MnO_3 are studied. The method used resonant x-ray photoemission spectroscopy allows to select the contributions of the various components in the valence bands (VB). We can study not only the ground state, but also the lifetime of the excited (a core-level hole – VB electron) state, determine energies of the VB single-particle states and two-hole states at selected atoms, see reactions to sudden appearance of the core-level photo-hole. Fig. 1 shows the VB XPS spectra obtained at different photon energies *hf* crossing the core-level excitation thresholds. On Gd $N_{4,5}$ edge 148 eV the 8.5 eV peak increases in $GdNi_4Cu$. The Gd 4*d* core-level electron transfers to a long-lived Gd 4*f*-state, then the reverse transition occurs, accompanied by emission of an electron detected. Note that the peak is enhanced much more (350 times) on the Gd M_5 absorption edge (1184 eV). The nickel and copper spectra behave otherwise. The VB signal (0 – 9 eV) in $GdNi_3Cu_2$ does not change at the Cu L_3 excitation edge *hf* = 932 eV, but the Auger line appears with a starting binding energy of 14 eV. This means that the Cu 2*p* – 3*d* excited state very quickly leaves the parent atom and then the Auger decay occurs, forming two holes in the Cu 3*d*-states. Subtracting energy of two single-hole states (2·3.5 eV) from 14 eV, we find experimentally the interaction energy for two holes on the copper atom 7 eV. Nickel (panel $GdNi_5$) behaves the same as copper, but its Auger line is significantly broader than the appropriate copper line. Broadening is due to shaking or the multiple creation of electron-hole pairs near the Fermi energy upon the sudden occurrence of the photo-hole. The probability of this process on a nickel atom is very high, since the Ni has high density of 3d-states at the Fermi level. Shaking on the copper atom is much smaller, since the Cu 3d-states are deepened by 3.5 eV.

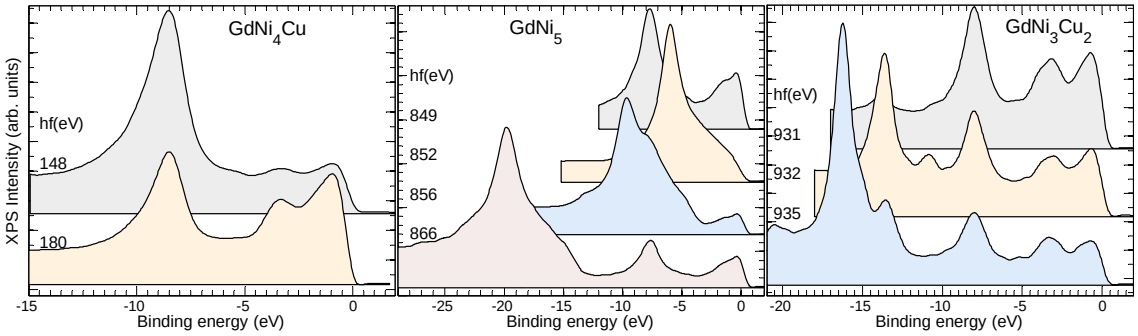

Fig. 1.

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On the Nature of Electron Localization in the High Pressure Phase of $LuFe_2O_4$

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ABSTRACT

$LuFe_2O_4$ invoked excitement several years ago after being identified as a mixed-valence compound with charge order (CO), meaning that a Fe^{2+} — Fe^{3+} — … superstructure prevails. It was initially concluded that this leads to ferroelectricity (FE), which originates from the mixed valence behavior and consequent charging of the single sheet components of the Fe-based bi-layers (these stack along the *c*-axis in the rhombohedral structure) [1]. Individual sheets comprise a triangular network of Fe atoms in the *a*-*b* plane. Ferrimagnetic ordering in this spin frustrated low dimensional system (2-D type lattice structure) is onset at T_M ~240 K. The claim for site-centered CO near ambient conditions as well as that this is the first case of electronically driven FE is a matter of controversy [1]. Nevertheless recent work demonstrates that this material has useful reversible oxygen storage capacities [2].

Previous pressure studies show that an irreversible rhombohedral (LP) → orthorhombic (HP) structural phase adjustment occurs at 5 – 8 GPa. There is also a large change in the pressure dependence of the room-temperature resistivity values as this pressure range is exceeded [3]. This new HP phase is fully stabilized at pressures above ~12 GPa. It may be recovered to ambient conditions and electron diffraction studies evidence Bragg satellites, supposed to be indicative of a new CO state associated with this HP phase.

We have employed ^{57}Fe Mössbauer effect (ME) spectroscopy at variable cryogenic temperatures to elucidate the magnetic-electronic state of the HP phase, by way of in-situ investigations in a diamond anvil pressure cell (DAC). This is a direct probe of the Fe valence state under extreme (pressure) conditions.

The results of this study indicate that the magnetic ordering temperature in the new HP phase is elevated to above room temperature. Spin frustration in the LP phase is relieved in the HP polymorph. The magnetic hyperfine fields and isomer (chemical) shifts evidence valence separation $Fe^{(2+\delta)+}$ — $Fe^{(3-\delta)+}$; but this deviates appreciably from ionic values, that is, $\delta > 0$. The HP phase nevertheless remains insulating, with resistivity values of recovered material one order of magnitude lower than the LP phase at ambient conditions. These results combined are suggestive of some degree of electron deconfinement in the magnetic HP phase. Is this then a case of Zener polarons and bond-centered CO, similar to what has been claimed in the mixed-valence manganites ?

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Fermi Surface Mapping and Pseudo-gap of Quasi-one-dimensional $Tl_2Mo_6Se_6$

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ABSTRACT

$Tl_2Mo_6Se_6$ is a linear chain compound consisting of molecular chains Mo_3Se_3 on a hexagonal lattice and Tl guest ion in between. It is the most 1-dimensional superconducting material with a transition temperature T_c > 5K discovered [1]. We have measured the Fermi surface map, showing that the band structure is even more 1-dimensional than predicted by density functional calculations. The spectral weight close to E_F is reduced, indicative of a pseudo-gap, but at the k_F a single sharp peak is found thus ruling out spin-charge separation as would be expected for a Luttinger liquid. The results from this single-band compound will be compared to the expected band structure of the multi band $K_2Cr_3As_3$ [2, 3].

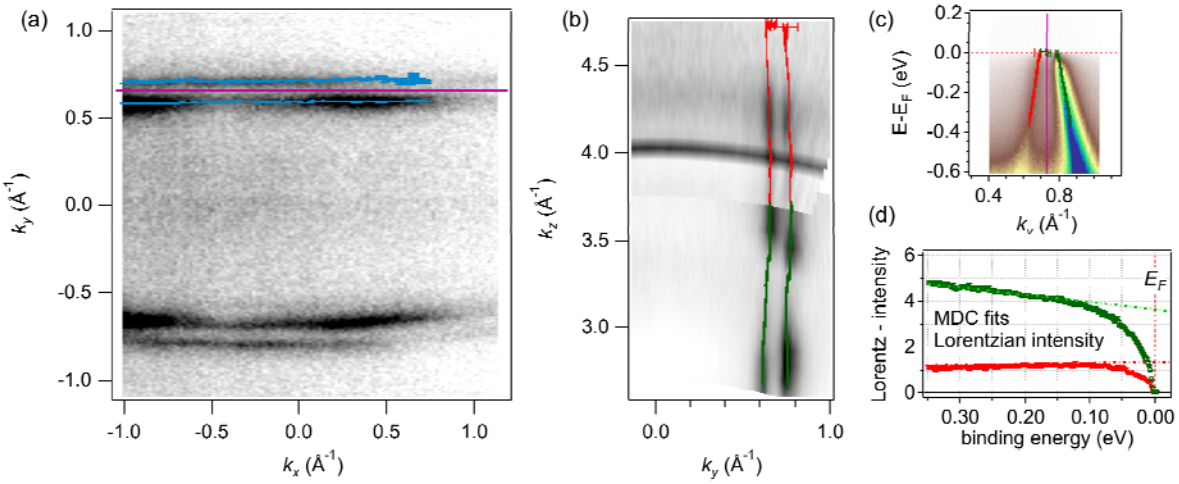

Fig.1 (a, b) ARPES Fermi surface maps of $Tl_2Mo_6Se_6$ as a function of k_x k_y *and* k_z, where *y* is along the chains, *x* is across, in the sample plane and *z* is across out of the sample plane. Peak positions of fits of two Lorentzian functions to the momentum distribution curves (MDC) are overlaid in part of the image. The Brillouin zone boundary, inferred from these peak positions, is indicated as a line that serves as a guide to the eye. Note that the curvature in (b) as well as the arc close to k_z = 4 Å^{-1} are artifacts of the measurement. (c) ARPES dispersion cut along at the (arbitrarily defined) k_x = 0 and k_z = 3 Å^{-1}. (d) Intensities extracted from the fits to the MDCs, straight dashed lines serve to show the spectral weight depletion (pseudo-gap) close to E_F.

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Angle-resolved Photoemission Spectroscopy of Correlated Electron Pairs in NiO and CoO

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ABSTRACT

It is well perceived that the independent electron approximation breaks down in strongly correlated materials. Therefore, there is a keen interest to develop a direct experimental probe to spectroscopically resolve the characteristic feature of electron correlation in these materials. One way is to explore the double photoemission (DPE) spectroscopy where an photoelectron pair is excited by a single photon, and the energy as well as the angular distribution of photoelectron pairs can be investigated [1].

In this contribution we present energy- and angle-resolved DPE on NiO and CoO films using a laboratory high-order harmonic generation light source in combination with time-of-flight spectrometers [2]. We use a photon energy of 25 eV and measure the distribution of photoelectrons in an energy window from 2 eV to 17.5 eV. In the two-dimensional energy spectra of the photoelectron pairs on both of these materials, the distribution of photoelectron pairs depends dominantly on the sum kinetic energy of the pair (E_{sum}). At higher E_{sum} the DPE intensity decreases and vanishes at about E_{sum} = 13 eV. This maximum sum kinectic energy of pairs can be quantitatively estimated by the electronic structure [3] and is attributed to emission of two *d* electrons from the top of the valence band. Moreover, the DPE intensity at a given sum energy shows a constant distribution as a function of the energy difference between the two photoelectrons in the pair. We further compare the DPE spectra on these oxides with a transition metal Ag, and the importance of *d* electrons for electron correlation will be discussed.

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Possible Mechanisms of Carrier Localization, Metal–insulator Transitions and Stripe Formation in Inhomogeneous Hole-doped Cuprates

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ABSTRACT

Possible mechanisms of carrier localization, metal–insulator transitions (MITs) and stripe formation in inhomogeneous hole-doped cuprates have been studied theoretically. Three distinctly different scenarios are proposed for the carrier localization in three-dimensional (3D) lightly doped cuprates in which the self-trapping and pairing of hole carriers (i) near the small-radius dopants and (ii) in a defect-free deformable lattice lead to the formation of the extrinsic and intrinsic (bi)polaronic states in the charge-transfer gap of the cuprates, and (iii) the self-trapping of carriers away from the largeradius dopants results in the formation of the in-gap hydrogenic impurity states. The binding energies and radii of the extrinsic and intrinsic large (bi)polarons in cuprates are calculated variationally using the continuum model and adiabatic approximation. We have shown that the extrinsic and intrinsic 3D large bipolarons exist in lightly doped cuprates at $\eta = \varepsilon_\infty/\varepsilon_0 < 0.127$ and $\eta < 0.138$, respectively, where $\varepsilon_\infty(\varepsilon_0)$ is the optic (static) dielectric constant. While the optical bipolarons can exist if $\eta < 0.134$ and the Fröhlich coupling constants a are greater than 5.8. The dopant- and carrier-driven inhomogeneities favor the specific charge ordering in the form of a 3D network of carrier-rich and carrier-poor stripes and the formation of different superlattices and in-gap bands of dopants and large polarons. The localized in-gap states develop into metallic states at some critical doping levels. We use the uncertainty relation to obtain the specific conditions for the Mott, Anderson and new MITs in cuprates. The applicability limits of these MITs in cuprates are clarified. We argue that the new MITs in the cuprates caused by the strong carrier–defect–phonon and carrier–phonon interactions are accompanied by the formation of a 3D self-organized network of carrierpoor (insulating) and carrier-rich (metallic) stripes, which coexist in a wide range of doping $x \approx 0.02\text{-}0.20$, and the suppression of superconductivity observed in underdoped region near the $x = 1/8$ is caused by the formation of insulating stripes on a global scale and by the preponderance of insulating phase compared with the metallic one. Our results are in good agreement with the existing experiments on *La*-based and other cuprates.

Fermi Surface Topology of Superconducting β-Bi_2Pd: ARPES and DFT Studies

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ABSTRACT

Among the Bi-Pd alloys there are several superconducting materials that crystallize in various structural phases having different transition temperatures, one of them is β-Bi_2Pd that has tetragonal structure (space group *I*4=*mmm*) with a T_c of ~4.5 K.
Measurements of the temperature dependences of the upper critical magnetic field and the specific heat suggest that β-Bi_2Pd might be a multi-band superconductor [1].
However, recent low temperature STM study has shown existence of the single s-wave superconducting gap (T_c=4.6 K) with the BCS-like temperature dependence of the superconducting gap in the weak coupling limit (Δ/k_BT_c=1.76) [2].

We have used angle-resolved photo-emission spectroscopy (ARPES) together with density functional theory (DFT) calculations to explore the electronic structure of this new superconducting material β-Bi_2Pd. We will be able to map out the full three-dimensional Fermi surface of β-Bi_2Pd by performing detailed measurements of the electronic structure as function of k_z. We compare these experimental results with our theoretical predictions as well as previous calculations [3].

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A Quantum Confined Gas of Large Polarons at the $SrTiO_3$(001) Surface

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ABSTRACT

The two-dimensional electron gas (2DEG) at the interface of the band insulators $LaAlO_3$ and $SrTiO_3$ has become a central figure in the emerging field of oxide electronics. The 2DEG is known to reside entirely in $SrTiO_3$ and combines high carrier mobility with properties such as gate-tuned superconductivity and magnetism that are not found in conventional semiconductor 2DEGs [1]. Understanding these properties has been hampered by the lack of experimental information on the underlying many-body interactions. In the context of superconductivity, electron-phonon interaction is of primary interest. Coupling to $SrTiO_3$ phonon modes has also been invoked to explain the dramatically increased superconducting transition temperature of monolayer FeSe grown on the $SrTiO_3$(001) surface [2].

Here we present a high resolution ARPES study of electron-phonon coupling in the 2DEG supported by the bare $SrTiO_3$(001) surface, which has the same electronic structure as the interface 2DEG [3]. *In-situ* surface preparation permits unprecedented control over the number of carriers confined to the (001) surface allowing us to trace the evolution of the electron-phonon coupling as a function of carrier density. In the low-density regime of the 2DEG we observe replica bands and a pronounced mass enhancement at the Fermi level. This is characteristic of an itinerant polaronic state arising from strong coupling to the 100 meV longitudinal optical phonon with low momentum transfer. As we increase the density we find a decreasing coupling strength and eventually a crossover to a regime with moderate and nearly uniform coupling to the entire phonon density of states, which we attribute to increased electronic screening.

Our results provide a microscopic basis for the modeling of transport properties including superconductivity in $SrTiO_3$-based heterostructures and demonstrate how surface and interface engineering can be used to tune many-body effects in transition metal oxides.

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Charge-density-wave Transition in LaAgSb2 Investigated by Angle-resolved Photoemission Spectroscopy

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ABSTRACT

The RAgSb2 family (R= rare earth) exhibits highly anisotropic electronic and magnetic properties correlated to the anisotropic atomic structure. In LaAgSb2, anomalies in the resistivity and magnetic susceptibility have been observed[1]. X-ray diffraction experiments have provided evidence of a Peierls transition that accounts for these anomalies[2]. X-ray scattering measurements evidence a periodic charge and lattice modulation below 207K along the a direction of tetragonal structure. Further lowering in temperature, an additional CDW ordering was observed along the c direction. Here we report the modifications of the Fermi surface as a function of the temperature using high resolution angle-resolved photoemission spectroscopy (ARPES).

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Angle-resolved Photoemission Study of a Thermoelectric and Multiferroic Delafossite $CuCrO_2$

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ABSTRACT

A delafossite-type oxide $CuCrO_2$ is a multi-functional oxide which has potential for a high-performance thermoelectrode, a *p*-type transparent conducting oxide, and a multiferroic material [1]. In view of a candidate for a thermoelectrode, when hole carriers are doped into the system, the electron density of states at the Fermi level (E_F) should rapidly change in order to yield a large Seebeck coefficient. Such an electronic structure is theoretically expected to be formed by the "pudding mold"-like band dispersion at the top of the valence band in a typical thermoelectric material $NaCoO_2$ [2]. To examine potential for the high thermoelectricity in $CuCrO_2$, the detailed momentum-dependent electronic structure near E_F has to be clarified. Here, we performed angle-resolved photoemission spectroscopy (ARPES) of $CuCrO_2$.

ARPES measurements were carried out at the beamline BL-28A of Photon Factory, KEK, using a Scienta SES 2002 electron analyzer with the photon energy of 80 eV. We succeeded in observing the band dispersion in $CuCrO_2$ for the first time, which can qualitatively be explained by a first principles band structure calculation study [3]. The near-E_F band dispersion (the binding energy of <1 eV) was found around the boundary of the hexagonal Brillouin zone, which is dominated by the Cr 3*d* state [1,3]. This band dispersion is relatively flat along the K-M line but is very fast along the Γ-K and Γ-M lines. In addition, we found that the flat dispersion approaches E_F toward the K point, indicating that the "pudding mold"-like dispersion is realized at the K point in $CuCrO_2$. Thus, from the view point of the electronic structure, we confirmed that doped holes in the present material, which has the Cr 3*d*-like character, can play a role for the high thermoelectricity.

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ARPES Study of Electronic Properties of In-situ Grown Ultra Thin $NdNiO_3$ Films in Proximity to a Magnetic Underlayer

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ABSTRACT

A compound from the RNiO3 family of strongly correlated oxides, $NdNiO_3$ (NNO) exhibits metal to insulator transition-MIT that is accompanied by simultaneous magnetic and charge orders [1,2]. To understand the role of magnetism on electronic structure of NNO we performed temperature dependent high-resolution angle-resolved photoemission spectroscopy (ARPES) study on perturbed electronic/magnetic structure of the ultra-thin film of NNO.

ARPES is a very surface sensitive technique which potential we fully utilized in combination with pulsed laser deposition (PLD). This approach gives satiated control of the measured system. By using PLD, a bilayer systems consisting of underlying magnetically ordered film of $La_{1-x}Sr_xMnO_3$($La_{1-x}Ca_xMnO_3$) and ultrathin film of NNO (2-5 u.c.) was created. By changing the content of Sr(Ca) we can control magnetic ordering in the manganite layer from ferromagnetic metallic (x=0.33 , FM/M) to antiferromagnetic charged ordered one (x=0.66, AF/I). We perform high resolution ARPES to map the electronic structure $NdNiO_3$ films in 3D k-space as a function of the temperature.

Obtained study gives important information about the influence of magnetic orders on the electronic structure and correlation effects in nickelates, with the potential to have a big impact on the field.

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Large Energy-scale ARPES Spectral Modulation with Temperature in a Layered Manganite

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ABSTRACT

A layered manganese oxide $La_{2-2x}Sr_{1+2x}Mn_2O_7$ (x=0.4) is widely known for its extraordinary property, the colossal magnetoresistance (CMR) effect, which is a manifestation of a ferromagnetic metal-to-paramagnetic insulator transition in zero field. Although the double-exchange (DE) mechanism can explain the basic physics of CMR (and this metal-insulator transition (MIT)), it fails to describe its magnitude, for explanation of which many investigations have been performed. In parallel with the MIT, drastic changes in the electronic structure near the Fermi level (E_F) with temperature (T) should be expected and have been observed indeed [1,2]. They observed vanishingly small quasi-particle spectral weight in very limited k-space regions centred at k_F accompanied by large incoherent spectral weight, both weight of which show large changes with T. In particular, the change in the quasi-particle spectral weight with T was found to scale to the change in the electrical conductivity [2]. However, more changes over the near-E_F region have also been observed (mostly) in cubic perovskite-type manganese oxides since decades ago [3], which has not been discussed enough so far.

In order to examine the large energy-scale changes and their k-space dependence, we performed T-dependent angle-resolved photoemission spectroscopy (ARPES) study of $La_{2-2x}Sr_{1+2x}Mn_2O_7$ (x=0.4) for the whole valence-band region. The measurements were carried out at the beamline BL28-A of Photon Factory, KEK, using a SES-2002 electron analyzer. We observed T-dependent spectral weight shift and modulation not only in the e_g band near E_F but also in the t_{2g} band located at 2-3 eV and even in the bottom of the valence band at ~7 eV. With increasing T, the $d_{x^2-y^2}$ band near the Γ point approaches E_F in agreement with the DE mechanism, while the $d_{3z^2-r^2}$ band moves in the opposite direction. The intensity modulation of the bottom of the valence band seems to be linked to that of the t_{2g} band. All these changes can consistently be interpreted as the large modulation of Mn 3d-O 2p hybridization across the MIT.

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Significant Doping Effect in the Annealing Process and True Phase Diagram of Electron Doped Cuprate

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ABSTRACT

High T_c superconductivity (SC) in cuprates is induced by introducing holes and electrons to the anti-ferromagnetic (AF) mother compounds. Although Sr and Ce substitutions provide enough holes and electrons for the La-214 cuprate family, annealing in low oxygen atmosphere is necessary to develop SC, especially in the electron doped side. It is believed that the heat treatment reduces the amount of impurity and thus SC appears. In fact, it was recently reported that impurity free samples were obtained through a 'protective annealing'. [Ref.1]

However, in addition to the impurity issue, doping effect needs to be considered as another key ingredient in understanding the SC in these systems. This is because oxygen acts as an anion and removing oxygen can induce additional electron doping. For this reason, we have investigated the doping effect of the annealing process by exploiting the Luttinger sum rule. Systematic ARPES studies were performed on single crystalline $Pr_{1-x}LaCe_xCuO_{4\pm\delta}$ or PLCCO (x=0.1, 0.15 and 0.18) prepared with various annealing conditions. Upon oxygen removal, we observe significant deviation in the doping concentration from the nominal doping determined by the Ce content. We find that PLCCO can reach heavily over doping up to x=0.24 with a rather high T_c ~19K. This result demonstrates parity between phase diagrams of hole- and electron-doped cuprates, at least on the over-doped side. In addition, we estimated the impurity effect and successfully constructed a phase diagram of superconducting and AF states by simultaneously considering the real doping and impurity. In this presentation, I will introduce the new phase diagram for PLCCO as a function of the true doping (estimated from the Luttinger sum rule) and impurity rather than the old phase diagram based on Ce content only.

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Momentum Dependence of a Kondo Resonance in $Ce_2Co_{0.8}Si_{3.2}$

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ABSTRACT

$Ce_2Co_{0.8}Si_{3.2}$ is a nonmagnetic Kondo lattice system with Kondo and coherence temperatures estimated to be 50 K and 80 K, respectively. It has enhanced specific heat, which amounts to C/T=200 mJ/($mol_{Ce}K^2$) at 0.4 K. Below 10 K an evidence of Griffiths phases was found [1].

ARPES studies of $Ce_2Co_{0.8}Si_{3.2}$ were conducted along Γ(M) – A(L) at T= 25 K [2]. They revealed nondispersing Kondo resonance (KR) with its spin-orbit splitting partner and dispersing bands. The experiment revealed two bands crossing Fermi energy (E_F), one of which has a parabolic shape and a surface character. The second one forms an electron pocket near the Γ point. KR shows a considerable variation of the intensity as a function of wave vector (k). Its maximum is found at the k-vector, where a band crossing E_F is observed in FPLO calculations but not in the experiment. This is not the first situation for cerium intermetallics, where KR is well seen while the corresponding band is not detected by ARPES [3]. We interpret the band dependence of the KR intensity as an evidence of strongly anisotropic hybridization between 4f electrons and conduction band, which was predicted theoretically [4-6] for cerium systems.

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Polaronic Effects in 3D Systems and Buried Heterostructures Explored by Soft-X-ray ARPES

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ABSTRACT

Spectroscopic power of soft-X-ray ARPES (SX-ARPES), employing photon energies around 1 keV, arises from enhanced photoelectron escape depth, sharp definition of 3D electron momentum **k**, and resonant photoexcitation delivering elemental and chemical state specificity. During the last few years this technique has pushed from bulk crystals to the most photon-hungry cases of buried interfaces and impurities [1]. We report applications of SX-ARPES to polaronic metal systems including 3D materials and buried interfaces.

The perovskite $La_{1-x}Sr_xMnO_3$ is a paradigm 3D polaronic metal system exhibiting CMR properties. Competition between the double-exchange related electron itineracy and polaronic self-trapping leads to its crossover from Fermi liquid in the ferromagnetic state to poorly conducting polaronic metal in the paramagnetic state. The experimental band structure of $La_{1-x}Sr_xMnO_3$ monocrystals, resolved by virtue of sharp 3D momentum definition of SX-ARPERS, confirms the GGA+*U* picture without any polaronic pseudogap typical of the bilayer manganites, consistently with decrease of electron-phonon coupling with dimensionality. The experimental Fermi surface (FS) unveils the canonical topology of electron spheres and hole cubes. Their shadow contours reminiscent of those in cuprates manifest the rhombohedral lattice distortion, as confirmed by one-step photoemission calculations. The distortion is neutral to the Jahn-Teller effect and thus polaronic coupling, but reduces the double-exchange electron hopping and thus the magnetoresistive T_c.

First applications of SX-ARPES to polaronic physics of buried heterostructures is illustrated with the $LaAlO_3/SrTiO_3$ interface. Ultrahigh energy resolution and variable X-ray polarization have enabled resolution of separate d_{xy}-, d_{yz}- and d_{xz}-derived subbands in the interface quantum well. Different Fourier composition of these bands modulates their ARPES response through **k**-space. The characteristic peak-dip-hump spectral lineshape manifests strong polaronic coupling of the interface electrons, immediately reducing their mobility. The polaronic hump blows up with temperature, explaining the mobility drop above 200K. The phonon spectrum change around 100K reflects the cubic to tetragonal phase transition in $SrTiO_3$. Oxygen vacancies progressively increase the electron concentration, as expressed by the Luttinger count of the experimental FS, and reduce the polaronic coupling strength.

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Soft X-ray ARPES Study of the New Diluted Magnetic Semiconductor $Ba_{1-x}K_x(Zn_{1-y}Mn_y)_2As_2$

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ABSTRACT

The newly-found diluted magnetic semiconductor (DMS) $Ba_{1-x}K_x(Zn_{1-y}Mn_y)_2As_2$ is isostructural to the "122"-type iron-based high-temperature superconductors and has a ferromagnetic Curie Temperature (T_C) as high as 230 K [1]. This material has an advantage that the charge reservoir Ba layer and the ferromagnetic ZnAs layer are separate, allowing us to independently control the amount of hole carriers and magnetic ions by substituting K for Ba and Mn for Zn, respectively. In addition, the substitution of Mn atoms for isovalent Zn atoms enables us to circumvent the problem of the low chemical solubility encountered in $Ga_{1-x}Mn_xAs$ and related DMSs, and makes it possible to obtain bulk crystals. X-ray photoemission studies on polycrystalline samples indicated that the Mn 3d partial density of states is quite similar to that of $Ga_{1-x}Mn_xAs$ [2].

Recently, $Ba_{1-x}K_x(Zn_{1-y}Mn_y)_2As_2$ bulk single crystals were successfully synthesized. In this work, we have investigated its electronic structure using single crystals with T_C = 60 K (x=0.3, y=0.15) by soft X-ray angle-resolved photoemission spectroscopy (SX-ARPES). Resonance SX-ARPES results suggest that the Mn *3d* split-off impurity band state near the Fermi level was not clearly observed unlike in $Ga_{1-x}Mn_xAs$.

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Electronic Entanglement and Classical Correlation in SmB_6

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ABSTRACT

We have analyzed the electronic structure of the strongly correlated material SmB_6 at 100 K using Density Functional Theory combined with Dynamical Mean Field Theory and Exact Diagonalization. The calculated spectral density is in good agreement with angular resolved x-ray photoemission data[1], including the size of the hybridization gap. The low-energy many-body eigenstates of the impurity Hamiltonian are analyzed in detail, with focus on their degree of entanglement[2]. The resulting intermediate valence ground state is both classically correlated (mixed) and quantum correlated (entangled) which makes the analysis of its topological properties[3] and surface states[1] more involved.

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Double Photoemission Spectroscopy on Silver and *3d* Transition Metal Oxides

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ABSTRACT

Electron correlation plays a critical role in various peculiar phenomena such as Kondo resonance, metal-to-insulator transition and high-temperature superconductivity. Meanwhile, exclusively due to the correlation between electrons, it is possible to excite an electron pair by one single photon in the so-called double photoemission (DPE) process. As recently outlined by theories, there exists a straightforward connection between the DPE cross-section and the strength of electron correlation in materials [1]. DPE spectroscopy therefore may become an unprecedented access to the electron correlation in a similar way as conventional angle-resolved photoelectron spectroscopy (ARPES) for the single-particle electronic structure.

In this contribution we present DPE experiments using two independent laboratory setups in order to address the general characteristics of electron correlation in solids. In one setup we use a home-built high-order harmonic generation light source in combination with time-of-flight spectrometers [2], and in the other we use a commercial He discharge lamp and hemispherical analyzers [3]. By comparing DPE experiments on Ag, NiO and CoO in both apparatuses, we observe higher DPE intensities from these oxides and provide indication for their stronger electron correlation. We further characterize the photon energy dependence in the observed DPE intensity. In the photon energy range from 18 to 48 eV, the DPE intensity is generally higher on NiO and CoO than on Ag. The onset of DPE from Ag is observed near the photon energy of 20 eV, whereas DPE on NiO and CoO starts at lower photon energies. Moreover, in the photon energy range investigated, the DPE intensity from NiO and CoO is comparable and this is in agreement with their similar strength of electron correlation expected from theories. Our results suggest a general experimental approach to probe the complex electron correlation in various solids and may allow a quantitative comparison with theories.

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Laterally Anisotropic Quantum Well States at the Surface of Anatase TiO_2 (001) Thin Film Unveiled by Angle Resolved Photoemission

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ABSTRACT

Anatase TiO_2 has attracted tremendous interest due to its potential applications in catalysis, photoelectrochemical solar cells, memristors, and as a transparent conductive oxide[1]. Recently, angle-resolved photoemission spectroscopy (ARPES) measurements on anatase TiO_2 surface by S. Moser and co-workers revealed a 3D metallic state with the formation of large polarons at low carrier density[2]. Here we report ARPES study of anatase TiO_2 (001) thin films grown *in-situ* using pulse laser deposition (PLD). We find that exposing the surface to synchrotron light it creates a metallic state with a high carrier density. The electronic structure consists of multiple subbands that derive from Ti $3d_{xy}$ orbital only. The n=1 subband shows a pure 2D character with no signs of dispersion along k_z. In addition, we observe folded bands due to the commonly observed (4×1) surface structural reconstruction on anatase TiO_2 thin films. The carrier density of both primary and folded bands increases with irradiation dose, and it saturates when bands extend to ¼ of Brillouin zone. Simultaneously, we observe an energy gap opening of ~ 20 meV along (0, 0) to (π, 0) direction. Our results open new avenues for manipulating electronic properties of anatase TiO_2 and new possibilities for its technological applications.

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Three-dimensional Electronic Structures of Layered Perovskite Iridates Studied by Ir-5d-sensitive ARPES

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ABSTRACT

The strong spin-orbit (SO) interaction of electrons contributing to the low-energy physics induces intriguing phenomena in the bulk in 5*d* transition-metal compounds. The Ruddlesden-Popper-phase strontium iridate $Sr_{n+1}Ir_nO_{3n+1}$ shows a variety of quantum phases such as the SO-Mott/Slater insulator and correlated metal depending on *n* or its structural dimensionality[1]. Although both Sr_2IrO_4 (*n*=1) and $Sr_3Ir_2O_7$ (*n*=2) are antiferromagnetic insulators, the electronic structures are found to be different from one another[2,3].

In order to shed light on the SO-driven exotic states, we have investigated three-dimensional electronic structures in the ***k*** space of the layered perovskite iridates Sr_2IrO_4 and $Sr_3Ir_2O_7$ by using soft-x-ray angle-resolved photoemission spectroscopy (SX-ARPES). The SX-ARPES experiments were performed at BL23SU in SPring-8, which have higher sensitivity for Ir 5*d* states relative to O 2*p* states than the vacuum-ultraviolet (VUV) ARPES. Despite the relatively poor energy and angular resolutions, SX-ARPES provides reliable information on the j_{eff} bands owing to the high Ir-5*d* photoelectron intensity in conjunction with high bulk sensitivity in the soft x-ray region.

The electronic structure of $Sr_3Ir_2O_7$ along the k_z axis is strongly modified by the Ir-O bilayer coupling while it resembles that of Sr_2IrO_4 in the k_x-k_y plane. In addition, we have observed in $Sr_3Ir_2O_7$ at *T*=80 K the significant photoelectron intensity on the chemical potential at (π, 0) point, which was not seen in Sr_2IrO_4. These results show up the unique nature of $Sr_3Ir_2O_7$ and the difference of electronic structures between these two iridates. They are even qualitatively different from the results of VUV-ARPES and provide a deeper insight into the physics of the novel correlated electron systems.

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Bond Stretching Phonon Softening and Kinks in the Angle-resolved Photoemission Spectra of under Doped $La_{2-x}Ba_xCuO_{4+\delta}$ Superconductors

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ABSTRACT

In the high-temperature (Tc) cuprate superconductors, a growing body of evidence suggests that charge ordering competes with superconductivity [1-3]. However, in cuprates such as $La_{2-x}Ba_xCuO_4$ (LBCO) and $La_{2-x-y}Nd_ySr_xCuO_4$ (LNSCO), whether the charge-modulations favor or compete with superconductivity, and their effect on the electron-phonon coupling are not yet understood, although an effect of the stripe order on the Cu-O bond-stretching mode is observed. We investigated the electronic structure of a $La_{2-x}Ba_xCuO_{4+\delta}$(LBCO) sample which displays simultaneously high temperature superconductivity and well defined Cu-O bond stretching softening, possibly due to the charge order instability. We find a kink in the band dispersion at a constant energy over the entire Fermi arc, at an energy matching the one of the softened Cu-O bond stretching phonon. Moreover, supposing that the scattering of this mode with the charge carriers quasi-particles is at the origin of the observed ARPES kink we also find a good match with the wave-vectors range of this mode softening.

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High-resolution Angle-resolved Photoemission Study of Fe/MgO(100)

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ABSTRACT

The oxygen adsorbed iron surface, Fe(100)-*p*(1×1)-O (O-Fe), is stable and used as a target material for the high-efficiency spin detector [1]. The surface states on pure Fe(100) and O-Fe related to transport properties have been examined by spin-resolved or spin-integrated angle-resolved photoemission spectroscopy (ARPES) [2,3]. However, information on the Fermi surfaces and band dispersions in thorough surface Brillouin zone (SBZ) with higher energy and momentum resolutions are still missing.

In this study, we have successfully performed high-resolution polarization-dependent ARPES experiments at HiSOR BL-1, examined the surface electron states of both pure Fe and oxygen adsorbed O-Fe films grown on MgO(100).

We measured Fermi surfaces and band dispersions with the p- and s-polarization geometries in thorough SBZ with high energy and momentum resolutions. We found that the band dispersions become significantly narrower and sharper after the oxygen adsorption than those in pure Fe. The measured Fermi surface mapping around $\bar{\Gamma}$ point of pure Fe and O-Fe taken at hv=55 eV. While the Fermi surfaces become sharper and clearer after oxygen adsorption, there exist similarities between pure Fe and O-Fe. There are several square-like Fermi surfaces around the $\bar{\Gamma}$ point of the SBZ for O-Fe, corresponding features can be found in pure Fe.

We found that major spectral features around the $\bar{\Gamma}$ and $\bar{M}$ points did not change depending on the incident photon energies for Fe and O-Fe, suggesting that these bands are surface-derived. We also examined the band dispersion around $\bar{M}$ point with improved energy resolution, and found that two kinks exist at -75 meV and -20 meV in the energy band dispersion.

Those results, comparing with previous experimental and theoretical studies, could give us more detailed information to understand the Fe(100) transport properties.

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The Spectral Function of Honeycomb Na_2IrO_3 by ARPES upon Li and Ru Substitution

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ABSTRACT

In recent years iridium oxides have received the attention of the scientific community owing to the strong interplay between spin-orbit coupling, one-electron hopping, and Coulomb repulsion. This unique combination of several comparable energy scales makes this class of compound extraordinarily interesting for studying correlated electronic phenomena. Particularly noteworthy is the small-gap antiferromagnetic insulator Na_2IrO_3, consisting of honeycomb $NaIr_2O_6$ layers stacked along the monoclinic c-axis, separated by hexagonal Na_3 layers [1]. A description of the electronic structure of this system has been proposed in terms of the splitting of the Ir-t2g manifold – due to spin-orbit interaction – into a doublet with effective angular moment J_{eff} = ½ and a quartet with J_{eff} = 3/2. The half-filled J_{eff} = ½ band at the chemical potential is further split into lower (LHB) and upper (UHB) Hubbard bands by electronic correlations (U), resulting in the so-called relativistic Mott insulating behavior. This scenario is validated by the observation of a 340meV conductivity gap open well above the long-range AFM ordering temperature T_N=15K [2]. Given the correlated nature of this system, further insights on the electronic properties might be obtained studying by ARPES the evolution of the low-energy spectral function upon substitution at the Na as well as Ir site, with Li and Ru respectively. This will be complemented by in situ alkali-adatom deposition to disentangle the evolution of microscopic interactions from simple charger-carrier doping effects.

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Layer-by-layer Study of the Interplay between Spin-orbit Interaction and Structural Distortions in Sr_2RuO_4

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ABSTRACT

The band structure and Fermi surface of Sr_2RuO_4, as determined by ARPES, are far more complex than what is expected from density functional theory calculations for the bulk material. This complexity has been shown to arise from a surface-to-bulk progression of the electronic structure originating from structural distortions in the surface [1] and subsurface layers [2], in synergy with spin-orbit interaction [3]. This leads to a complex and strongly $k_{||}$ and k_z dependent spin-orbital entanglement of the electronic wave function [3], as confirmed by spin-resolved ARPES experiments [4]. The normal state of Sr_2RuO_4 is now further investigated by means of polarization and photon-energy dependent ARPES measurements, aiming at obtaining layer-resolved information about the symmetry of the electronic states. Complementary to the experimental results, a spin- and orbitally-resolved *ab initio* based tight-binding modelling of the electronic structure, and corresponding ARPES intensity, is utilized to disentangle – layer-by-layer – the interplay between spin-orbit interaction and symmetry-breaking structural distortions.

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ABSTRACTS

Friday, July 10th, 2015

CORPES15

Friday, July 10th

Chairpersons: A. Tejeda, J.P. Rueff

IT-EX-23	Electronic structure and electron dynamics in two-dimensional materials *P. Hoffman*
IT-EX-24	Discovery of Weyl semimetal TaAs *H. Ding*
OC-TH-24	Topological phases at oxide interfaces: Material-specific insight from DFT+DMFT *O. Janson*
OC-EX-25	Non-topological 2DEG at the surface of YbB_6 and divalent hexaborides *J. Denlinger*
IT-EX-25	Spin polarization of surface states probed by ARPES *H. Ebert*
OC-EX-26	Complete determination of molecular orbitals by measurement of phase symmetry and electron density *A. Schöll*
OC-EX-27	First nanoARPES user facility available at SOLEIL: An effective band structure probe in nanoscience *C. Chen*

Electronic Structure and Electron Dynamics in Two-dimensional Materials

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ABSTRACT

Changing the dimensionality of a material results in significant modifications of its electronic properties. This is even the case if the parent material already has a layered structure with little interaction between the layers, as in the case of graphene, bilayer graphene and single-layer transition metal chalcogenides.

While the static electronic properties of novel two-dimensional materials can be studied by standard angle-resolved photoemission (ARPES), investigations of the ultrafast carrier dynamics require both time- and angular resolution and thus time-resolved (TR)-ARPES. There is, moreover, the technical requirement of high photon energies since the interesting part of the aforementioned materials' electronic structure (i.e. the (gapped) Dirac cone) is placed at the two-dimensional Brillouin zone boundary. Recently, it has become possible to probe states at such high *k* by TR-ARPES, thanks to the arrival of ultrafast high harmonic laser sources.

Here we characterize the dynamic processes around the Dirac point in epitaxial mono- [1] and bilayer [2] graphene, as well as around the band gap of single layer MoS_2 [3] using TR-ARPES, thereby addressing the timescales of hot carrier scattering processes in these systems. For bilayer graphene, we are able to disentangle the dynamics in the two conduction band sub-states and find that the gap in the lower sub-state plays a crucially important role, leading to a remarkably different relaxation dynamics compared to monolayer graphene.

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Discovery of Weyl Semimetal TaAs

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ABSTRACT

Weyl semimetals are recently predicted a class of materials that can be regarded as three-dimensional analogs of graphene breaking time reversal or inversion symmetry. Electrons in a Weyl semimetal behave as Weyl fermions, which have many exotic properties, such as chiral anomaly and magnetic monopoles in the crystal momentum space. The surface state of a Weyl semimetal displays pairs of entangled Fermi arcs at two opposite surfaces. However, the existence of Weyl semimetals has not yet been proved experimentally. Here we report the experimental realization of a Weyl semimetal in TaAs by observing Fermi arcs formed by its surface states using angle-resolved photoemission spectroscopy. Our first-principles calculations, matching remarkably well with the experimental results, further confirm that TaAs is a Weyl semimetal.

Topological Phases at Oxide Interfaces: Material-specific Insight from DFT+DMFT

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ABSTRACT

Continued efforts to discover new topological states of matter in real materials recently brought oxide heterostructures to the forefront of the field. In these artificial materials, the charge, orbital and spin degrees of freedom can be manipulated to an unprecedented degree, allowing for a controlled tuning of the physical properties. Since the fabrication of heterostructures is generally challenging, the search for candidate materials is largely delegated to the computational methods. Despite the complications arising from strong electronic correlations, recent studies demonstrate that the formation of topological states can be traced back to their microscopic roots, in a quantitative agreement with the experiment [1].

One of the most promising candidates for the emergence of topological phases are (111) perovskite bilayers, where the correlated atoms form a distorted honeycomb lattice [2]. The case in point are $LaAlO_3$-$LaNiO_3$ (111) interfaces based on Ni^{3+}, with one electron in the e_g orbital manifold. A recent DFT+*U* study predicted a sizable orbital polarization for 1/1 (alternating Ni and Al layers) interfaces. For the Ni-bilyars, the same study predicts the band gap opening accompanied by a ferromagnetic ordering, leading to a multiferroic behavior [3]. Here, we further explore the properties of $LaAlO_3$-$LaNiO_3$ (111) interfaces by considering purely local as well as cooperative Jahn-Teller distortions and taking dynamical electronic correlations into account. We study the nature of the Mott transition and the role of magnetic correlations. In addition, we eventuate the topological indices following the recently developed approaches for strongly correlated systems.

This work has been supported in part by European Research Council under the European Union's Seventh Framework Programme (FP/2007-2013)/ERC through grant agreement n. 306447.

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Non-topological 2DEG at the Surface of YbB_6 and Divalent Hexaborides

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ABSTRACT

Both a recent theoretical prediction that YbB_6 is an *f-d* band-inverted mixed-valent topological insulator (TI) very similar to SmB_6 [1] and subsequent topological interpretations of V-shaped electron pockets [2-4] observed in angle-resolved photoemission spectroscopy (ARPES) are at odds with the previous experimental classification of the material as a divalent small *p-d* band gap semiconductor.

Our ARPES studies of the (001) surface of YbB_6 confirm the nearly pure divalency of Yb and demonstrate that in-gap surface electron pockets, with slightly non-parabolic dispersion indicative of a small p-d gap, originate from quantum well (QW) states confined to the inversion layer of *n*-type and *p*-type surface regions with cation or boron termination. Proof of the QW origin of these states comes from (i) the relative energies of the $\bar{\Gamma}$, and $\bar{X}$, electron pockets, in agreement with 1D Poisson-Schrödinger simulations, and (ii) photon-dependent spectral intensity profiles that reflect the deep bulk sampling depth of the 2D states.

Spatial and temporal variations [5] of the effective surface charge and band bending potential fully explain both the observation of different electron pocket energies in the various ARPES measurements [2-5] and reports of Dirac-cone-like overlap of electron and hole features. Intentional surface charge modification via K-dosing provides a means to tune the band bending towards a spatially uniform *n*-type limit. Aged surfaces exhibit persistent QW hole states indicating the possibility of robust *p*-type band bending in air.

All of the observed behaviors for YbB_6, and also CaB_6, SrB_6 and EuB_6, are shown to be universal polar-surface-driven features of the divalent hexaborides, which also rules out another TI scenario of 4*f* spin-orbit enhanced *p-d* overlap gapping [3], since non-*f* CaB_6 has a well-established ≈1 eV band gap. Also DFT+U+SO+mBJ theoretical band calculations, using appropriate *f*-correlation energy U and the modified Becke-Johnson (mBJ) exchange potential, are able to reproduce the experimental energy ordering of a *p-d* gap existing at E_F above the Yb 4*f* states, without the *f-d* or *p-d* band inversions necessary for a TI scenario.

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Spin Polarisation of Surface States Probed by ARPES

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ABSTRACT

Angle-resolved photo emission in the UV-regime is a well established tool to investigate the electronic properties of surface states. A very promiment example for this are the topological surface states (TSSs) in three-dimensional insulators. Recent experimental and theoretical investigations in this field on the possibility to probe the spin polarisation of the TSSs by the use of circularly polarised light [1] has been extended by a detailed study on the impact of finite temperatures [2]. Because of the relatively low mean free-path length in the UV-regime these experiment however probe the surface near parts of the TSSs. By performing calculations based on the one-step model of photo emission, it is demonstrated that working at photon energies in the X-ray regime it is possible to obtain more detailed and complete information on the TSSs. This holds in particular concerning their spatial extend towards the bulk. As corresponding experiments are strongly affected by thermal vibrations these have been accounted for when calculating the spectra. This way favorable conditions for the various proto-type TI materials could be identified giving a helpful guide for corresponding experiments.

The magnitude of the spin polarization at the Fermi level of ferromagnetic materials at room temperature is a key property for spintronics. Accordingly, as a second example for the investigation on the spin polarisation of surface states results of a corresponding study will be presented. Investigating the Heusler compound Co_2MnSi a value of 93 % for the spin polarization has been observed at room temperature, where the high spin polarization is related to a stable surface resonance in the majority band extending deep into the bulk. In particular, we identified in our spectroscopical analysis that this surface resonance is embedded in the bulk continuum with a strong coupling to the majority bulk states. The resonance behaves very bulk-like, as it extends over the first six atomic layers of the corresponding (001)-surface. Our study complements experimental investigations, where the bulk electronic structure as well as surface-related features have been investigated using spin-resolved photoelectron spectroscopy (SR-UPS) and for a larger probing depth spin-integrated high energy x-ray photoemission spectroscopy (HAXPES). The corresponding results are discussed on the basis of first-principles band structure and photoemission calculations which consider all relativistic, surface and high-energy effects properly.

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Complete Determination of Molecular Orbitals by Measurement of Phase Symmetry and Electron Density

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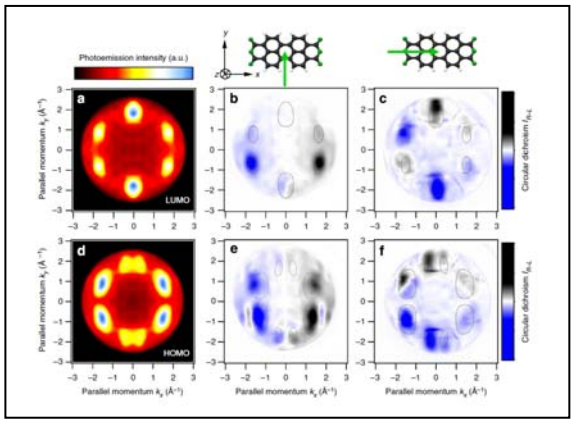
ABSTRACT

Several experimental methods allow measuring the spatial probability density of electrons in atoms, molecules and solids, that is, the absolute square of the respective single-particle wave function. In recent years Angle resolved photoelectron spectroscopy (ARPES) has emerged as a particularly powerful tool for the imaging of orbital densities [1,2]. But it is an intrinsic problem of the measurement process that the information about the phase is generally lost in the experiment. The symmetry of this phase, however, is a crucial parameter for the knowledge of the full orbital information in real space.



We demonstrate that the phase symmetry can be derived from an experimental approach from the circular dichroism in the angular distribution of photoelectrons. In combination with the electron density derived from the same experiment, the full quantum mechanical wave function can thus be determined experimentally [3].

We furthermore show that the mixing of molecular orbitals with delocalized substrate states leads to very interesting phenomena in these hybrid systems [4]. As a consequence the molecules communicate laterally via the substrate resulting in dispersing hybrid bands [5]. The localized character of the molecular states manifests itself in very sharp excitation features at the Fermi level, which can be explained by a generalized Kondo scenario [6,7].

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First NanoARPES User Facility Available at SOLEIL: An Effective Bandstructure Probe in Nanoscience

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ABSTRACT

In recent decades, we have witnessed exponential advances in a wide diversity of the new nanotechnologies. These advances, seen particularly in nanoelectronics, nanomagnetism and nanochemistry, among others, affect almost every aspect of our lives. Following the fundamental step in the creation of nano-objects and even if these "building blocks" have shown remarkable properties, they would have remained unexploited if, at the same time, we had not developed new tools capable of analyzing, viewing and scrutinizing objects on a wide range of scales, from a few microns to a few tens of nanometers.

Recently, great progress has been made as a result of the rapid expansion in the range of modern microscopies. However, if they have achieved nanometer spatial resolution, the challenge still remains to provide powerful high-energy-resolution spectroscopic tools for probing nano- and micro-areas. The challenge then, is to quantify and analyze the electronic properties of advanced materials on a nano- and mesoscopic-scale. For such a result, analysis of the electronic structure must be comprehensive, not only with regard to detection of core levels, but especially to study the structure of electronic states of the valence bands, directly responsible for chemical bonds, electrical transport and the thermal and mechanical properties.

In order to fill this need, we have recently developed a novel X-ray microscope, labelled, nanoARPES (Nano Angle Resolved Photoelectron Spectroscopy), particularly well-suited to provide valuable spectroscopic and electronic information in the real and reciprocal space of mesoscopic samples. It is a cutting-edge technique able determining the momentum and spatial resolved electronic structure of advances materials at the nano- and meso-scale[1-6].

In this presentation, the latest unpublished results of the ANTARES microscope beamline of SOLEIL will be disclosed. In particular, nanoARPES findings describing the electronic band structure of mono-atomic thick graphene films grown on insulating substrates will be presented. This end-station, with a spatial resolution of several tens of nanometers, has already been able to carry out direct imaging of core levels, their chemical shifts and the band electronic structures of several ordered materials and their derived heterostructures. High precise Chemical images and valence band information of nano-objects like exfoliated grapheme, granular materials and Nanowires will be disclosed in detail.

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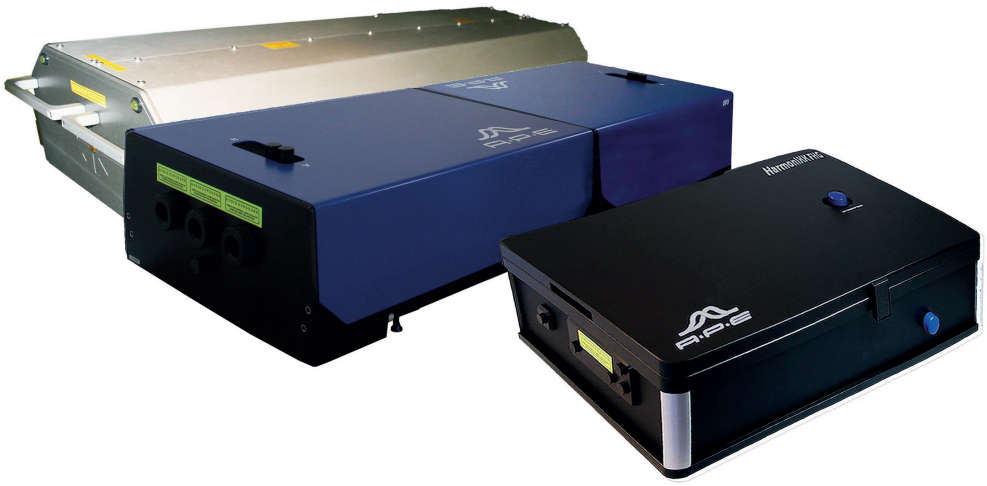

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- Wavelength range < 192 ... 215 nm (> 6.45 ... 5.76 eV)
  210 ... 230 nm (5.90 ... 5.39 eV)
  230 ... 320 nm (5.39 ... 3.87 eV)
- High pulse repetition rate (80 MHz)
- For photoelectron spectroscopy
- For UV Raman spectroscopy

Angewandte Physik & Elektronik GmbH

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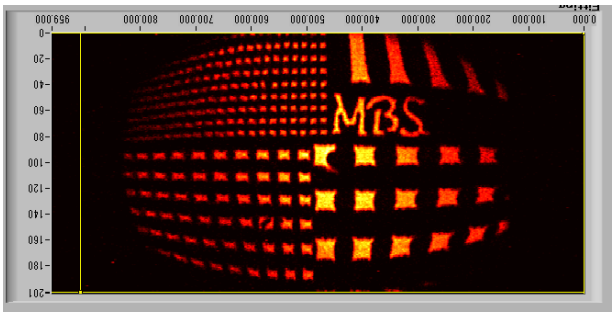
Do you use ARPES measurements?
Do you want to analyse Spin component?

Our state of the art
ARPES System with 2D Angular mapping (new!)
MBS A-1SYS + L4 lens



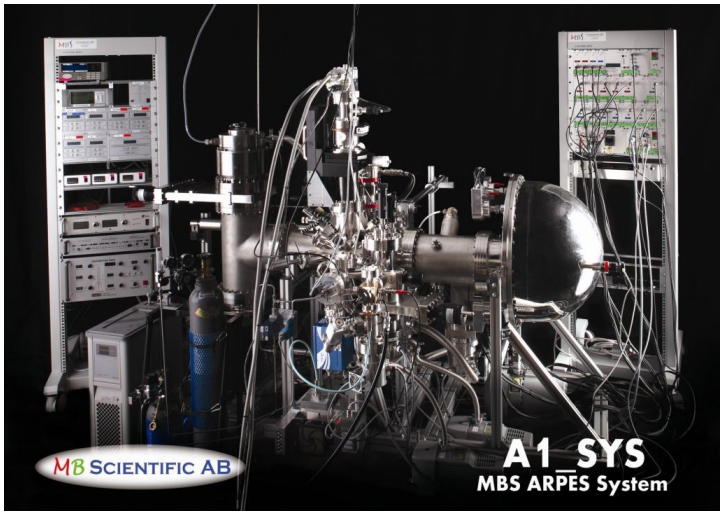
2D Angular mapping data taken by MBS A-1_#0022 analyser with L3_AS lens.

Furthermore developed L4 lens is now ready for you!

This 2D (35 * 20 degree) ARPES image is taken about a half minutes!!

ARPES System with 3D VLEED Spin detector
MBS A-1SYS + MBS 3D-VLEED

Gives you the results!



For the detailed information please contact us!

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e-mail: info@mbscientific.se **Home page:** www.mbscientific.se

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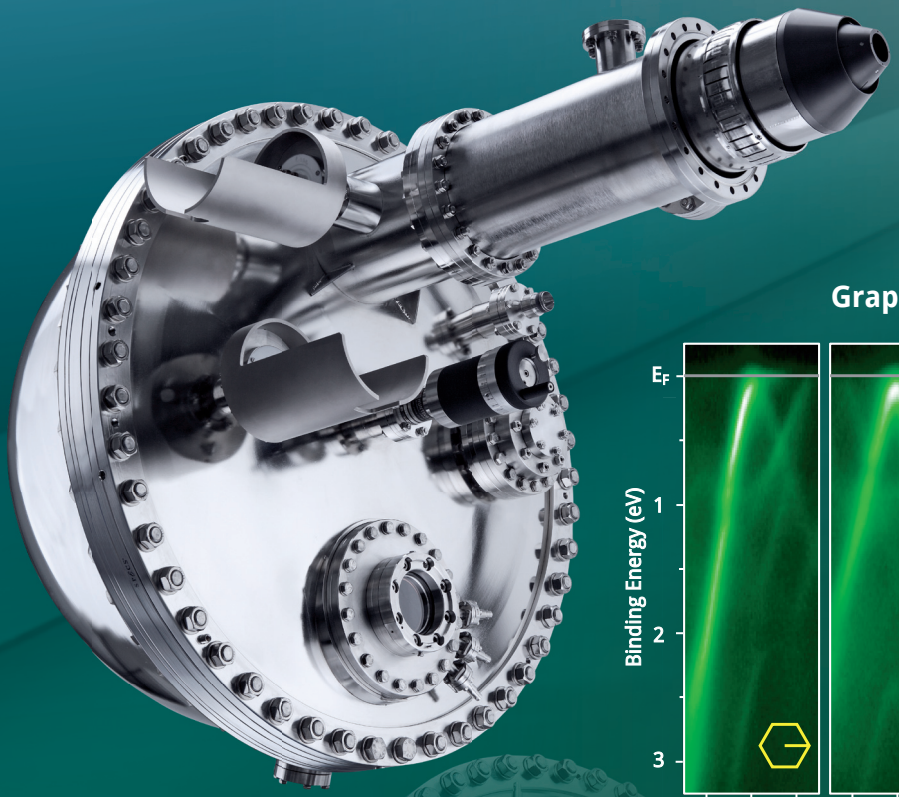
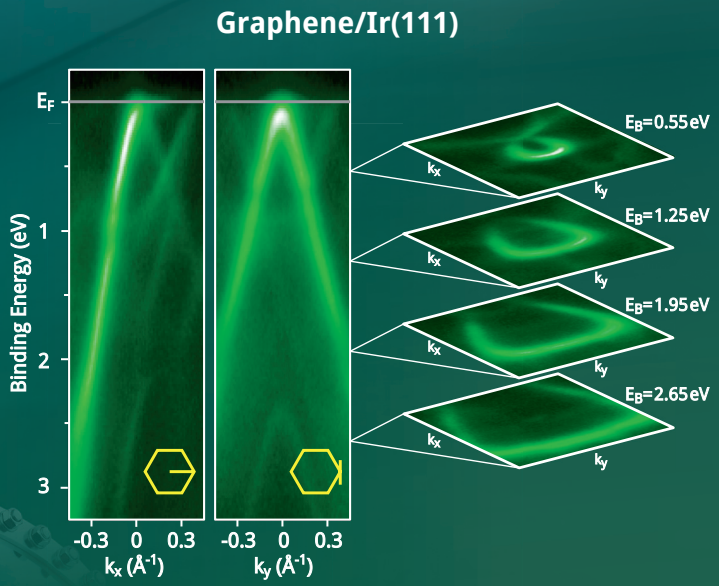
FOR ULTRA HIGH RESOLUTION
ARPES AND HAXPES

KEY FEATURES

- Ultra High Energy Resolution in UPS (<1 meV)
- Angular Mapping (Δθ < 0.1°)
- Different Modes of Operation (UPS, XPS and HAXPES)
- CCD, DLD and DLD/SPIN Detection Available





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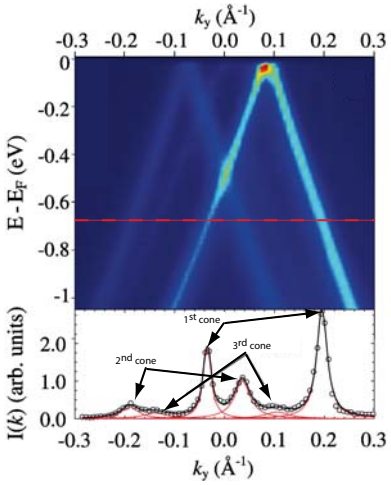
VG SCIENTA HIGHLIGHTS

GRAPHENE

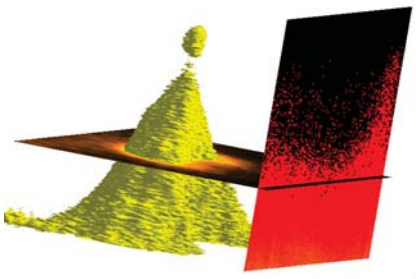
ARPES provides direct access to the electronic structure of materials. This makes the technique ideal for studying systems with novel electronic properties, e.g. graphene.

ARPES ON GRAPHENE



Left) Top) ARPES spectrum of intersecting Dirac cones of graphene grown on SiC(000-1). Bottom) Momentum dispersion curve from top image, as indicated by the red dashed line. For more information see M. Sprinkle PRL 103 (2009) 226803. Data courtesy of Amina Taleb-Ibrahimi at the Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, Gif sur Yvette, France and Ed Conrad at GeorgiaTech, Atlanta, USA. **Right)** Scienta R4000 state-of-art analyser.

SCIENTA ARTOF 10K - FULL K-PARALLEL ACCEPTANCE



Left) Electronic stucture of graphene recorded with fixed manipulator position using the full k-parallel detection of Scienta ARTOF 10k. Data courtesy: A. Lindblad, R. Ovsyannikov (private communication, 2012). **Right)** Scienta ARTOF 10k analyser.

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