Trendoxides 2015

Workshop program

Monday, Nov. 14th. Aula Magna, via Trieste 17

09:00 **Jean-Marc Triscone**: *Magnetic coupling through lanthanum nickelate in non-metallic $LaMnO_3/LaNiO_3$ heterostructures*

09:40 **Ralph Claessen:** *Photoemission of metallic states at $SrTiO_3$-based surfaces and interfaces: The role of oxygen vacancies*

10:10 **Vladimir Strocov:** *Electrons and polarons in TMOs and their interfaces explored by soft X ray ARPES*

11:00 **Giancarlo Panaccione:** *Critical thickness of electronic screening in LSMO thin films*

11.30 **Stefano Gariglio:** *The Superconducting Phase Diagram of $LaAlO_3/SrTiO_3$ Interfaces*

12:00 **Giovanni Drera:** *Beyond LAO-STO: probing functionalised oxides heterostructures with X-ray electron spectroscopies*

12.30 **Dana Popescu**: *Band alignment and charge reorganization at metal/ferroelectric interface*

Aula Magna, via dei Musei 41

14.30 **Mario Cuoco:** *Spin-orbital physics in hybrid oxides*

15:00 **Luca de' Medici** *The capricious electron correlation strength of transition metal oxides.*

15.30 **Massimo Capone:** *Ferroelectric Metals: Building Blocks for the design of high-temperature multiferroics*

16:00 **Francesco Peronaci:** *Transient Dynamics of d-wave Superconductors after a Sudden Excitation*

Brescia, November 16-18, 2015

Tuesday, Nov. 15th. Aula Magna, via Trieste 17

09:00 **Andrivo Rusidy**: *High-energy optical conductivity on oxide interfaces and correlated electron systems*
09:30 **Marc Golden** : *Verwey fast. Picosecond speed limit for switching in a complex oxide*
10:00 **Nicolas Bergeal:** *Quantum phase transitions at oxide interfaces*

11:00 **Giorgio Sangiovanni:** *Heterostructures with correlated electrons: examples from two Vanadium Oxides*
11.30 **Stefano Roddaro:** *Hybrid Graphene / Oxide Heterostructure Devices*
12:00 **Veljko Zlatic** *Thermoelectric properties of strongly correlated multilayers*
12.30 **Carlo Castellano**: *Evidence of local structural order and spin-lattice coupling in $Y_{2-x}Zn_xRu_2O_7$ pyrochlores*
12.45 **Marius-Adrian Husanu**: *Oxygen depletion in a ferromagnetic hole-doped manganite revealed by photoelectron spectroscopy and first principles calculations*

Aula Magna, via Trieste 17

14.30 **Giacomo Ghiringhelli**: *High Tc Cuprate Superconductors studied with Resonant Elastic and Inelastic soft X-ray Scattering*
15:00 **Adolfo Avella:** *Defects, Disorder, and Strong Electron Correlations in Orbital Degenerate, Doped Mott Insulators*
15.30 **Simone Peli:** *The room temperature prodrome of charge-order in copper oxides*

16.30 **Matteo Gatti** *Coupling of excitations: correlation beyond the quasiparticle picture*
17:00 **Francesco Randi**: *Phase separation in the non-equilibrium Verwey phase transition in magnetite*
17.15 **Lorenzo Malavasi:** *Origin od colossal magnetoresistance in LaMnO3 manganites*
17.45 **Chiara Bigi**: *Electronic properties of epitaxial hole/electron doped $La_{0.7}(Ba,Ce)_{0.3}MnO_3$ thin films by photo-emission spectroscopies*

Wednesday, Nov. 16th. Aula Magna, via Trieste 17

09:00 **Gianfranco Pacchioni:** *Two-dimensional oxides: from microelectronics to nanocatalysis*

09.40 **Alberto Verdini:** *Excess electrons distribution in TiO_2(110) and Mg:TiO_2(011) surfaces*

10.10 **Federico Cilento** *Time-resolved XUV photoemission: a new clue for understanding the ultrafast dynamics in copper oxides*

10.40 **Daniele Fausti:** *Disclosing fluctuations of lattice atomic positions by non-equilibrium optical experiments*

11.40 **Lorenzo Del Re**: *Non-equilibrium and non-homogeneous phenomena around a first-order quantum phase transition*

11.55 **Etienne Janod:** *Universal out-of-equilibrium insulator to metal transitions induced by electric field in Mott insulators*

12.25 **Mariela Menghini:** *Exploring the metal-insulator transition in pure and doped V_2O_3 (ultra)thin films*

12.55 **Michele Fabrizio:** *Non-Zener electric breakdown and other surprises near a first order Mott transition*

Mon 09:00 - Jean-Marc Triscone

Magnetic coupling through lanthanum nickelate in non-metallic $LaMnO_3/LaNiO_3$ heterostructures

M. Gibert[1], M. Viret[1,2], S. Catalano[1], J. Fowlie[1], P. Zubko[3], N. Jaouen[4], J.-M. Tonnerre[5], S. Gariglio[1] and J.-M. Triscone[1]

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Perovskite nickelates ($RNiO_3$, RE=Rare Earth) are fascinating materials, well known for their metal to insulator transition (MIT) and unique antiferromagnetic (AFM) ground state [1].
In this talk, I will discuss quite broadly why we are interested in the physics of complex oxide structures and interfaces. I will then explain how one can control the MIT and of the magnetic properties of high quality epitaxial films of nickelates through a variety of techniques [2-6].
I will then describe our work on heterostructures containing $LaNiO_3$ – the only member of the family that is metallic and paramagnetic in the bulk down to low temperature – and ferromagnetic $LaMnO_3$. We observed in this system an unusual exchange bias in [111] oriented ($LaNiO_3$)/($LaMnO_3$) superlattices [7] and an antiferromagnetic interlayer exchange coupling above the blocking temperature of the exchange biased state specifically in 7 unit cells / 7 unit cells superlattices. The antiferromagnetic coupling is attributed to the presence of a (1/4,1/4,1/4) wavelength AFM structure in $LaNiO_3$ – the complex exchange bias to this particular AFM structure and the presence of two types of interfaces [8].

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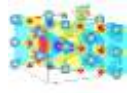

Mon 09:40 - Ralph Claessen

Photoemission of metallic states at $SrTiO_3$-based surfaces and interfaces: The role of oxygen vacancies

Ralph Claessen

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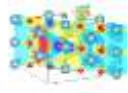
The insulator $SrTiO_3$ can host high-mobility two-dimensional electron systems (2DESs) on its surfaces and in interfaces with other oxides. While the metallicity of the bare surface is induced by oxygen vacancies (O_{vac}), it is believed that the interface 2DES in heterostructures like $LaAlO_3/SrTiO_3$ (LAO/STO) is caused by their polar discontinuity. Here I will discuss soft x-ray photoemission experiments of buried oxide interfaces and bare STO surfaces with precise in situ control of the oxygen stoichiometry, focused at the specific role of O-vacancies in these systems. Using resonant photoemission (ResPES) at the Ti L-edge we identify the simultaneous presence of itinerant and localized Ti 3d electrons, whose concentrations can be tuned by vacancy doping. It is demonstrated that the 2DES of the heterointerface has indeed an intrinsic component existing even in the absence of O-vacancies, in contrast to the case of the bare STO surface. For the spinelperovskite heterostructure γ-Al_2O_3/STO we find indications for a specific O-defect bound immediately to the interface. This situation is reminiscent of delta-doping and may be responsible for the extremely high 2DES mobility seen in this system. Finally, low-energy angle-resolved photoemision (ARPES) on Ovac-controlled STO surfaces provides evidence for a pronounced electronic inhomogeneity, which may be related to similar magnetic inhomogeneities ("ferromagnetic puddles") recently observed in the LAO/STO interface.

Work in collaboration with M. Sing, L. Dudy, G. Berner, J. Gabel, F. Pfaff, P. Scheiderer, P. Schütz, M. Zapf (all at U Würzburg), T.-L. Lee, C. Schlueter (Diamond Light Source), V.N. Strocov, C. Cancellieri (Paul-Scherrer-Institute/Swiss Light Source), H. Fujiwara, A. Sekiyama, A. Yamasaki, S. Suga, Y. Saitoh (U Osaka/Spring-8), and J.D. Denlinger (Advanced Light Source).



Mon 10:10 - Vladimir Strocov

Electrons and polarons in TMOs and their interfaces explored by soft-X-ray ARPES

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Angle-resolved photoelectron spectroscopy (ARPES) is a unique experimental technique to explore electronic structure of crystalline system resolved in electron momentum **k**. The spectroscopic power of soft-X-ray ARPES (SX-ARPES), employing photon energies *hv* around 1 keV, arises from increase of the photoelectron escape depth by a factor of 3-5 compared to the conventional VUV energy range, and resonant photoexcitation delivering elemental and chemical state specificity. The advanced instrumentation at the Swiss Light Source has in the recent years allowed SX-ARPES to develop from traditional applications to 3D bulk crystals to the most photon-hungry cases of buried interfaces and impurities [1] and, with recent progress in energy resolution, intervene into the domain of polaronic effects.

A precursor of the interface studies, applications of soft-X-ray ARPES to bulk materials use its intrinsically sharp resolution in 3D electron momentum **k** resulting from the enhanced photoelectron delocalization. One example is the strongly correlated TMO material $La_{1-x}Sr_xMnO_3$ having a 3D pseudocubic structure. Its experimental Fermi surface (Fig. 1) reveals, on top of the classical manifold of electron spheroids and hole cuboids, additional "shadow" contours resembling those in cuprates and manifesting the rhombohedral structural distortion [2]. In competition between the double-exchange delocalization and polaronic self-trapping, this distortion reduces the CMR critical temperature. Other examples of bulk TMOs include CrO_2 probed through amorphous Cr_2O_3 overlayer, etc. Our "drosophila" example of buried TMO interfaces is $LaAlO_3/SrTiO_3$ (LAO/STO) which embeds mobile 2D electron system exhibiting

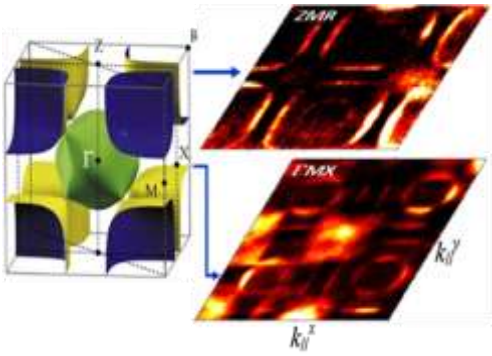

Fig.1. Experimental Fermi surface of the 3D perovskite $La_{1-x}Sr_xMnO_3$.

ferromagnetism, low-temperature superconductivity and other exotic properties. The ARPES response of the buried interface electrons can be accentuated using resonant photoexcitation of the interface Ti^{3+} ions at $h\nu \sim 460$ eV. Ultrahigh energy resolution of ~35 meV and variable X-ray polarization enable resolution of separate d_{xy}-, d_{yz}- and d_{xz}-derived subbands in the interface quantum well (Fig. 2*a*). The ARPES response of these bands, varying through **k**-space, reflects Fourier composition of their wavefunctions. Remarkably, the experimental (**k**-integrated) spectral function (Fig. 2*b*) shows a pronounced peak-dip-hump structure formed by the quasiparticle peak and its satellite hump. This lineshape manifests a polaronic state of the interface electrons caused by their coupling to hard LO3 phonons through strong electron-phonon interaction. This effect fundamentally limits mobility of the interface charge carriers and exhaustively accounts for the experimental m_{eff} renormalization without any notable effects of electron correlations [3]. Manipulation by oxygen vacancies, which inject extrinsic electron density and concomitantly reduce the polaronic coupling, opens ways to circumvent this fundamental limit and boost the interfacial mobility, critical for device applications. With increase of temperature, the quasiparticle weight dramatically reduces due to polaronic coupling to soft TO1 phonons [3]. This effect elucidates the microscopic mechanism behind the mysterious drop of interfacial mobility observed in transport. The LAO/STO interface realizes thus a polaronic metal state involving at least two phonons with different energies and thermal activity. The polaronic effects are actually typical of TMO perovskites, reflecting their highly ionic character and easy structural transformations. Other oxide heterostructures, including EuO/Si spin injectors, are also reviewed in this talk.

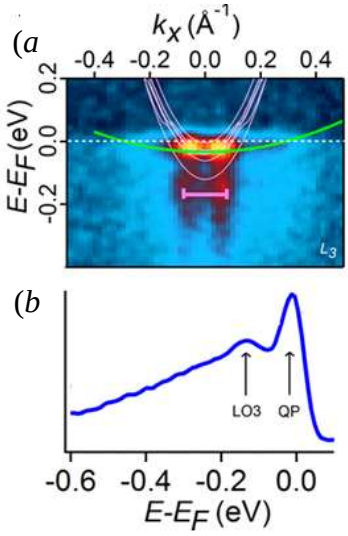

Fig.2. LAO/STO interface: (*a*) Experimental d_{xy} and d_{yz} band structure, and (*b*) spectral function identifying the polaronic state.

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Mon 11:00 - Giancarlo Panaccione

Critical thickness of electronic screening in LSMO thin films

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Unravelling what ultimately drives the electronic and magnetic properties of transition metal oxides (TMOs) is strictly linked to a direct measure of the electronic energy distribution of the metal orbitals [1]. A paradigmatic example is found in manganites, like $La_{0.66}Sr_{0.33}MnO_3$ (LSMO). The peculiar transport and electronic properties of LSMO thin films make them very attractive for spintronic applications and device-tailored interfaces [2]. Surface and interface effects are of utmost importance in this context, since it is well known that the electron correlations in TMOs are severely influenced by the surface environment (electronic/structural reconstruction, defects, etc.).
The enhanced probing depth of Hard X-ray Photoemission spectroscopy (HAXPES) has recently proven not only to overcome surface related effects but also to identify the presence of different screening mechanisms between the surface and the bulk electronic structure, revealing unique spectroscopic features [3-6], which are not visible with surface sensitive spectroscopies. We have shown that these additional features are signatures of both metallic and ferromagnetic properties [5,6].
We report on valence band and core level HAXPES results on well-characterized LSMO thin films grown by means of PLD and MBE at the APE-NFFA facility [7]. We have performed X-ray experiments (HAXPES, XAS, XMCD) vs. temperature and vs. strain (as induced by mismatch to different substrates). We were able to reveal: i) the critical thickness at which the truly bulk electron screening is set, confirming that the surface has different electronic properties, ii) a clear evolution in the valence band states vs. strain.

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Mon 11.30 - Stefano Gariglio

The Superconducting Phase Diagram of $LaAlO_3/SrTiO_3$ Interfaces

Stefano Gariglio[1], Alexandre Fête[1], Danfeng Li[1], Wei Liu[1], Margherita Boselli[1], Marc Gabay[2] and Jean-Marc Triscone[1]

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2 Laboratoire de Physique des Solides, Université Paris-Sud, Orsay Cedex, France

The discovery of a two-dimensional electron liquid (2DEL), formed at the interface between the two band insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO), has generated significant interest. The 2DEL has indeed intriguing electronic properties including superconductivity and spin-orbit interaction which can be tuned both by field-effect.
In this talk I will introduce the main electronic properties of this oxide interface before discussing in detail the low temperature phase diagram revealed by field-effect experiments. I will then compare the superconducting behaviour of this 2D system with the one of 3D doped STO crystals.

Mon 12:00 - Giovanni Drera

Beyond LAO-STO: probing functionalised oxides heterostructures with X-ray electron spectroscopies

Giovanni Drera

Interdisciplinary Laboratory for Advanced Material Physics (I-LAMP) and Mathematics and Physics Department, Università Cattolica del Sacro Cuore, Brescia (Italy)

The discovery of a two-dimensional electron gas (2DEG) at the interface between two perovskite oxides, i.e., lanthanum aluminate ($LaAlO_3$, LAO) and strontium titanate ($SrTiO_3$, STO) [1], has disclosed unexpected perspectives in the physics of oxide-based junctions. So far, a large number of studies have attempted to determine the physical properties of the 2DEG. In this context, X-ray photoelectron spectroscopies, such as standard XPS, resonant photoemission (ResPES) and hard X-rays photoemission (HAXPES) are powerful tool to investigate the junction physics. These techniques allow to map the electronic structure, to describe the junction band profile and to investigate the cationic disorder and stoichiometry with elemental selectivity. Nevertheless, an accepted explanation of LAO-STO interface physics is still hard to be found, because of the complex superposition of several issues typical of oxides heterostructures, such as structural roughening (interdiffusion), oxygen or cationic vacancies formation during or after the growth, substoichiometry, external doping sources or surface charge accumulation effects. In spite of the lack of consensus on the conductivity onset mechanism, the LAO-STO has already proven the feasibility of all-oxide electronic devices (FET), scaled down to submicrometer dimension[2].
Since the conduction in non-polar STO (given by the $Ti^{4+}O_2^{4-}$ – $Sr^{2+}O^{2-}$ layer stacking) seems to be related to the LAO polar nature ($La^{3+}O^{2-}$ - $Al^{3+}O_2^{4-}$ structure), several other trivalent perovskites, such as $LaGdO_3$, $LaCrO_3$, $NdGaO_3$, $LaGaO_3$ etc. are currently tested as an effective LAO replacement, with the aim to increase the junction functionalities by exploiting the peculiar oxide overlayer properties. A notable group of suitable perovskite materials are multiferroics, which simultaneously display ferroelectricity, ferromagnetism (or anti-ferromagnetism) and ferroelasticity. In this context, bismuth ferrite ($BiFeO_3$, BFO in short) is the only room-temperature single-phase multiferroic [3], with high ferroelectric Curie temperature (1103 K) and Neel temperature (643 K); BFO also shows a strong magneto-electrical coupling, which allows to reverse the magnetic order by changing the electric polarization and vice-versa. Such material grown on STO could in principle allow to finely tune the 2DEG density locally, for example through biased-tip microscopy technique (i.e, AFM and PFM), and thus to design switchable electrically lithographed devices operating at room temperature.
The first part of the talk will be devoted to the presentation of X-ray electronic spectroscopies results on conductive and insulating LAO-STO [4,5,6], with a strong focus on band junction diagram and cation diffusion effects probed by angle-resolved XPS. The

second part of this talk will be devoted to our recent results on BFO [7] and BFO:STO interfaces, grown by RF-sputtering; in particular, the possibility to use XPS as a tool for epitaxial growth quality assessment will be discussed. Finally, a preliminary band diagram for the BFO:STO junction will be presented.

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Work done in collaboration with: G. Salvinelli, A. Giampietri, C. Pintossi, F. Rigoni, and L. Sangaletti (Università Cattolica del Sacro Cuore, Brescia); F. Bondino, E. Magnano, S. Nappini, A. Verdini, L. Floreano, A. Cossaro (CNR-IOM, Trieste, Italy); J. Huijben, M. Huijben, G. Rijnders, D.H.A Blank, H. Hilgenkamp, A. Brinkmann (Twente University, the Netherlands); I. Alessandri (Mechanical and Industrial Engineering Department, University of Brescia).

Mon 12.30 - Dana Popescu

Band alignment and charge reorganization at metal/ferroelectric interface

D.G. Popescu [1*], M.A. Husanu[1]

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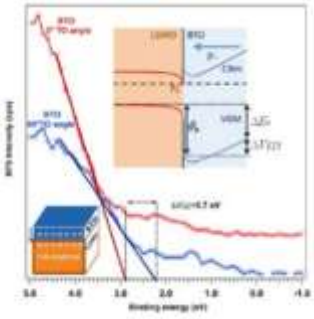
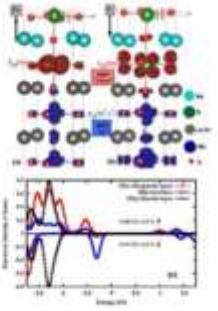
In a metal/ferroelectric junction there is usually a synergy between the band alignment at the interface region driven by the different work function of the two materials and the depolarization field which may be insufficiently screened by the metallic electrodes. This is reflected accordingly in variation of the valence band and core level positions which are not obvious to explain. There is also an influence on the symmetry of the bonding states which can be traced down in the ferrodistortive displacements of the interface atoms, with deep implications in modulating the conductance at the contact region. Our work addresses the effects of band alignment on the symmetry of the interface states for a prototypical M/FE interface: ferromagnetic $La_{0.6}Sr_{0.4}MnO_3$ covered by a ferroelectric (FE) $BaTiO_3$ layer. Using *ab-initio* calculations we deduce that the interface has antiferromagnetic character, with a significant spin polarization for the interface Ti atom which couples with the Mn atoms through a double exchange mechanism mediated by the apical oxygens. The height of the Schottky barrier of 1.25 eV estimated from photoemission data is compared with the calculated value using two different methods and a fair agreement is established.



Interface band alignment driven by ferroelectric polarization at the LSMO/BTO interface



Orbital polarization and interface antiferromagnetism

Mon 14:30 - Mario Cuoco

Spin-orbital physics in hybrid oxides

Mario Cuoco

SPIN-CNR and Dipartimento di Fisica 'E.R. Caianiello', Università di Salerno, I-84084 Fisciano (Salerno), Italy

Transition metal (TM) oxides are fascinating materials characterized by a subtle interplay between charge, spin, and orbital degrees of freedom, which in many cases gives rise to complex types of collective behavior. Though first thought as a prerogative of 3d systems this class of phenomena seems now to be ubiquitous in 4d and 5d ones. In this framework, we present how magnetic and orbital patterns in a uniform 4*d* host are modified by the inclusion of 3*d* impurities substituting the 4*d* ions for both insulating and metallic hosts.
In particular, for the case of an insulating host, we investigate the changes in spin and orbital patterns induced by magnetic transition-metal ions without an orbital degree of freedom doped in a strongly correlated insulator with spin-orbital order. In this context, we study the 3*d* ion substitution in 4*d* transition-metal oxides in the case of $3d^3$ doping at either $3d^2$ or $4d^4$ sites, which realizes orbital dilution in a Mott insulator. Although we concentrate on this doping case as it is known experimentally and more challenging than other oxides due to finite spin-orbit coupling, the conclusions are more general. We derive the effective 3*d*−4*d* (or 3*d*−3*d*) superexchange in a Mott insulator with different ionic valencies, underlining the emerging structure of the spin-orbital coupling between the impurity and the host sites, and demonstrate that it is qualitatively different from that encountered in the host itself. This derivation shows that the interaction between the host and the impurity depends in a crucial way on the type of orbital pattern. One finds that in some cases, due to the quench of the orbital degree of freedom at the 3*d* impurity, the spin and orbital order within the host is drastically modified by doping. The impurity either acts as a spin defect accompanied by an orbital vacancy in the spin-orbital structure when the host-impurity coupling is weak or favors doubly occupied active orbitals (orbital polarons) along the 3d−4d bond leading to antiferromagnetic or ferromagnetic spin coupling. [1]
For the case of a metallic host, we show that doping a t_{2g} system can lead to emergent orbitally directional double-exchange effects. We find that, due to the orbital directionality, the competition between antiferromagnetic (AF) and ferromagnetic (FM) correlations in layered systems makes antiferromagnetically coupled FM zigzag stripes and checkerboard clusters the dominant patterns in the phase diagram over a large range of doping. We demonstrate how the breaking of the orbital directionality as well as the inclusion of the Coulomb interaction can significantly affect the zigzag-checkerboard competition and lead to orbital or charge ordering in the ground state. [2]

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Mon 15:00 - Luca de' Medici

The capricious electron correlation strength of transition metal oxides

Luca de' Medici

ESRF, Grenoble (FR)

Hund's exchange coupling is a well-known main player (through Hund's rules) in the physics of isolated atoms and insulators. It was however recently shown that it has a crucial influence also on the dynamics of conduction electrons in correlated materials.
Taking this effect into account helps explaining the capricious dependence of electron correlation strength and the occurrence of Mott insulating states in transition metal oxides. Hund's coupling also favors a differentiation of correlation strength among conduction electrons, a potentially fertile ground for new phenomena in these materials, such as d-electron heavy-fermionic behavior.

Mon 15.30 - Massimo Capone

Ferroelectric Metals: Building Blocks for the design of high-temperature multiferroics

M. Capone (SISSA and CNR-IOM, Trieste, Italy)

The realization of a ferroelectric metal in which ordered electric dipoles coexist with metallic behavior may appear hard or even impossible because the itinerant electrons are expected to screen any electric dipole inside the material.
Fifty years ago, Anderson and Blount theoretically proposed how to overcome this contradiction [1]. A metal with polar distortions can realized if the inversion symmetry is broken displacing ions which are decoupled from the electronic states at the Fermi level [1,2].
Nevertheless, an unambiguous realization of this behavior was only found in 2013 in $LiOsO_3$, a metal with half-filled bands which shares many structural similarities with the ferroelectric insulator $LiNbO_3$ [3].
We show how another physical ingredient plays a central role in this material: the electron-electron correlations [4]. $LiOsO_3$ has indeed a half-filled Os-d manifold, a configuration which is particularly sensitive to electron correlations, as it can easily turn into a Mott insulator. Here the actual values of interactions are such that the material is almost on the brink of Mott localization, but it retains a â€œbadâ€• metallic character. Direct comparison with reflectivity measurements confirms the very poor metallic conduction of the material, which appears as crucial to let the polar distortions survive [5].
We then propose how to turn this non-magnetic polar metal into a multiferroic through the design of a superlattice, which increases the degree of correlation, leading to Mott localization of the Os orbitals [6].
In the final part of the talk I will add more pieces to the puzzle of the interplay between strong correlations and ferroelectricity briefly discussing how a polar metal can be obtained in ferroelectric metal and how a significant magneto-electric coupling can arise even when magnetism and polarization have different physical origin.

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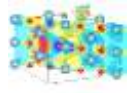

Mon 16:00 - Francesco Peronaci

Transient Dynamics of d-wave Superconductors after a Sudden Excitation

Francesco Peronaci,[1] Marco Schirò,[2] and Massimo Capone[1]

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Motivated by recent ultrafast pump-probe experiments on high-temperature superconductors, we discuss the transient dynamics of a d-wave BCS model after a quantum quench of the interaction parameter. We find that the existence of gap nodes, with the associated nodal quasiparticles, introduces a decay channel which makes the dynamics much faster than in the conventional s-wave model. For every value of the quench parameter, the superconducting gap rapidly converges to a stationary value smaller than the one at equilibrium. Using a sudden approximation for the gap dynamics, we find an analytical expression for the reduction of spectral weight close to the nodes, which is in qualitative agreement with recent experiments.

Tue. 09:00 - Andrivo Rusidy

High-energy optical conductivity on oxide interfaces and correlated electron systems

Andrivo Rusydi

Department of Physics, Faculty of Science, NSU, Singapore

Abstract: to appear soon

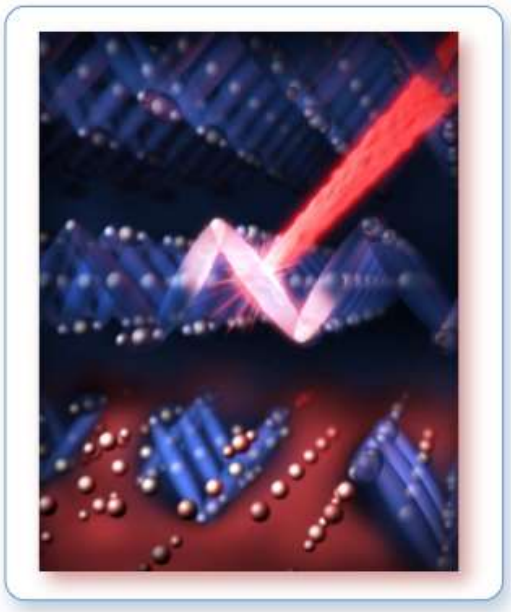
Tue. 09:30 - Marc Golden

Verwey fast. Picosecond speed limit for switching in a complex oxide

Mark S. Golden

Van der Waals-Zeeman Institute, IoP University of Amsterdam

For oxide electronics to come of age, we will need convincing that the dazzling array of physical properties transition metal oxides display can be switched on and off sufficiently rapidly. Femtosecond soft X-ray probes can clock such switching speeds, simultaneously laying bare the mechanisms at work by separating out the contributions from the lattice and electronic degrees of freedom on the time axis.
In magnetite - Fe_3O_4 - electrical conduction drops two-hundred-fold below T_V, as electrons freeze into a complex pattern of charge and orbitals, as first recognised by Verwey.



Harnessing the fs soft X-ray pulses from the Linac Coherent Light Source, it can be shown that, for all its complexity, the charge-orbital order of the insulating Verwey phase can give way to a metallic phase in as little as a single picosecond. This not only finally solves the riddle of the how the Verwey transition works, but also sets an encouraging speed limit in our pursuit of future oxide electronics technologies.

Artist's impression of the pump pulse annihilating trimerons in the Verwey phase, triggering the switching to a metallic phase.

S. de Jong, R. Kukreja et al., *Speed limit of the insulator–metal transition in magnetite*, Nature Materials 12, 882-886 (28 July 2013)

Tue 10:00 - Nicolas Bergeal

Quantum phase transitions at oxide interfaces

N. Bergeal[1], S. Hurand[1], J. Biscaras[1], J. Lesueur[1], C. Feulliet-Palma[1], R. C. Budhani[2], A. Dogra[3], M. Grilli[4], S. Caprara[4]

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At the interface between insulating oxides such as $SrTiO_3/LaAlO_3$ or $LaTiO_3/SrTiO_3$, a superconducting two-dimensional electron gas (2DEG) has been discovered [1-3], whose carrier density can be tuned by applying a gate voltage. Within the quantum well, a strong (a few meV) Spin Orbit Coupling has been measured. Using back and top gating, we recently showed that it is directly proportional to the electric field, as expected for a Rashba mechanism [4].
The unique possibility of modulating the superfluid density easily and continuously opens new perspectives to tackle fundamental issues in condensed matter physics, such as the Superconductor to Insulator Quantum Phase Transition (QPT) in a two-dimensional system.
Using two different external parameters, the magnetic field and the electric field, we explored the phase diagram of the 2DEG. As proposed theoretically [5], we point out that the system can be described as a disordered array of coupled superconducting puddles. Depending on the conductance, the observed critical behaviour is single (corresponding to the long-range phase coherence in the whole array) or double (one at intermediate distances belonging to the (2+1)D clean XY universality class related to local phase coherence, the other one to the array of puddles)[6]. Moreover, by retrieving the coherence-length critical exponent ν, we show that the quantum critical behaviour can be clean or dirty, depending on whether the phase-coherence length is smaller or larger than the size of the puddles.
Finally, the electric-field driven QPT reveals an anomalous critical behavior. It can be understood if we assume that the dynamics in the Cooper pair channel is dominated by critical dynamical density fluctuations in the low doping regime. This shades a new light on unexplained critical exponents found in the literature.

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Tue 11:00 - Giorgio Sangiovanni

Heterostructures with correlated electrons: examples from two Vanadium Oxides

Giorgio Sangiovanni*

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In this talk I will discuss two examples of correlated layered heterostructures: $SrVO_3$ thin films and $LaVO_3$ grown on $SrTiO_3$.
The latter turns out to be promising for photovoltaic applications [1] while the former has been proposed as a possible "Mott transistor" [2].
By means of Density Functional Theory and Dynamical Mean Field Theory we can single out the crucial role of the d-occupation in the physics of these and, more in general, of other correlated oxide heterostructures.

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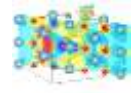

Tue 11.30 - Stefano Roddaro

Hybrid Graphene / Oxide Heterostructure Devices

Stefano Roddaro

Istituto Nanoscienze – CNR, NEST and Scuola Normale Superiore, Pisa (Italy)

Vertical stacks combining different layered materials offer novel opportunities for applications and fundamental studies. In my talk, I will give a brief overview of our work on the development of a new class of hybrid systems comprising single-crystalline monolayers of graphene [1] and LaAlO-SrTiO heterostructures [2]. The latter are known to support two-dimensional systems characterized by a set of interesting electric field-tunable properties, such as superconductivity [3], magnetism [4] and spin-orbit coupling [5]. Vertical heterostructures combining the two materials, in analogy to graphene/GaAs heterostructures [6], are expected to display a strong interlayer Coulomb coupling that can drive novel collective phases, and promise interesting device applications [7].

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Tue 12:00 - Veljko Zlatic

Thermoelectric properties of strongly correlated multilayers

Veljko Zlatic

Institute of Physics, Zagreb, Croatia

A theory of charge and heat transport in inhomogeneous multilayers (ML) with correlated electrons is presented. We consider a device which consists of several strongly correlated metallic mid-planes sandwiched between two semi-infinite Mott insulators. The chemical potential of the channel planes is tuned by the gate voltage which is perpendicular to the ML planes.

The charge and heat currents are parallel to the ML planes. The electron dynamics is described by a simplified Hubbard model which is solved, for large correlation, by the DMFT. When the system is doped away from the insulating phase, the low-energy slope of the renormalized density of states increases rapidly with the strength of the correlation. This can be used to generate a device with a very large figure-of-merit, ZT. The results for the electrical conductivity, the Seebeck coefficient, the power factor, the Lorenz number and ZT are presented. The effect of the number of planes is also discussed. Optimal tuning gives ZT >> 1.

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Tue 12.30 - Carlo Castellano

Evidence of local structural order and spin-lattice coupling in $Y_{2-x}Zn_xRu_2O_7$ pyrochlores

C. Castellano[1,*], G. Berti[2], S. Sanna[3], R. Ruiz-Bustos[4], J. van Duijn[5], A. Brambilla[2], Á. Muñoz-Noval[6], L. Duò[2], F. Demartin[1]

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The family of ruthenium pyrochlores $A_2Ru_2O(1)_6O(2)$ displays a high chemical and structural flexibility and as a consequence a wide range of chemico-physical properties like a metal-insulator transition, long-range ordering as well as spin-singlet transitions (1). As such they are also useful for specific applications (2-4). The wide variety of ground states is due to the fact that Ru can be either in the 4+ or 5+ oxidation state promoting good electro-catalytic properties. As a consequence, a very good electrochemical behaviour of Ru-based pyrochlores has been observed at temperatures as low as 350 °C, justifying their study as intermediate temperature solid-oxide fuel cell cathodes (5). In particular, $Y_2Ru_2O_7$ is characterized by rather large antiferromagnetic (AF) exchange couplings J among Ru^{4+} S=1 spins, giving rise to an AF phase transition at $T_N \sim 77$ K. We have performed magnetic susceptibility measurements showing a large zero field (ZFC)-field cooled (FC) deviation which suggests the presence of a spin-glass-like behaviour. To characterize in greater detail a potential magneto-structural coupling we have performed extended X-ray absorption fine structure measurements (EXAFS) at the Ru K-edge. On a local scale we found evidence of a significant magnetoelastic coupling at 77 K pointed out by a huge Debye-Waller σ^2 factor deviation from a correlated temperature dependent Debye-like local order behaviour plus a static contribution. Moreover, we noticed the occurrence of a never observed before potential local order-disorder structural phase transition at $T^* = 150$ K (6) consistent with the pyrochlores predisposition towards structural disorder and spin-phonon correlation. We have also studied the magnetic and structural properties of the A-doped $Y_{2-x}Zn_xRu_2O_7$ pyrochlore systems as a function

of the Zn^{2+} doping in the range $0.00<x<0.20$ (7). Magnetization and muon spin relaxation measurements show that the AF transition typical of the undoped compound is slightly reduced and broadened in the zinc doped samples. EXAFS measurements show a peak in the Ru-O(1) first shell Debye Waller factor at a temperature $T_{DW} \sim T_N$, giving evidence for a strong magnetoelastic coupling detected up to $x = 0.10$. A local precursor order-disorder transition at $T^* > T_N$ is also observed up to $x = 0.10$. For $x > 0.10$ these local structural features are hidden due to the increasing lattice distortion induced by the Zn^{2+} dopant whereas the magnetic transition is still present (7,8).

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Tue 12.45 - Marius-Adrian Husanu

Oxygen depletion in a ferromagnetic hole-doped manganite revealed by photoelectron spectroscopy and first principles calculations

Marius-Adrian Husanu[1,2], Dana G. Popescu[2]

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The effect of oxygen vacancies in a ferromagnetic $La_{1-x}Sr_xMnO_3$, x=0.4 hole-doped manganite is studied by correlated X-ray photoelectron spectroscopy and first principles calculations. The effects of defect oxygen vacancies are assessed by numerical calculations using explicit treatment of Sr doping. We find that the presence of Sr atoms is connected to the suppression of octahedral rotations. First principles calculations reveals that in LSMO, around the defect site, the magnetic moments of Mn atoms are enhanced locally with respect the nominal value of 3.6 μ_B to 3.8-3.9 μ_B without major effects on the states near the Fermi level. In X-ray photoemission we find evidence of ferrodistortive effects occurring at the LSMO surface whose signature is in turn identified in angle resolved photoelectron spectroscopy as surface resonance at a binding energy of ~0.3 eV due to subsurface Mn atoms.

Tue 14.30- Giacomo Ghiringhelli

High T_c Cuprate Superconductors studied with Resonant Elastic and Inelastic soft X-ray Scattering

Giacomo Ghiringhelli

CNISM, CNR/SPIN and Dipartimento di Fisica, Politecnico Milano, Italy

Layered cuprates form the most intriguing and intensely studied family of oxides. Their non-conventional superconductivity has motivated the application of all known experimental methods to gain a comprehensive description of their electronic and magnetic structure. The phenomenology has kept growing, in some cases to the benefit of a simpler general picture, in other cases just extending the catalogue of the exotic properties of these materials, thus complicating the puzzle by the addition of new tiles to the puzzle. In many cases cuprates have been the excuse for the development of new experimental techniques that have later been used on other materials.
In the recent years resonant soft x-ray scattering has provided exciting results both in the elastic (RXS) diffraction-like process, able to reveal charge ordering phenomena, and in the inelastic (RIXS) energy-loss spectroscopy, which contains information on the spin, lattice, orbital and charge excitations. In particular RXS has given the definitive evidence of charge density waves in the bulk of underdoped cuprates. And RIXS has demonstrated that damped spin excitations persist up to extreme overdoping.
I will briefly introduce the two techniques and present some key results , including spectra recently measured at the new ID32 beam line of the ESRF, equipped with the ERIXS spectrometer, and capable of 35 meV resolution for RIXS at the Cu L3 edge.

Tue 15:00 - Adolfo Avella

Defects, Disorder, and Strong Electron Correlations in Orbital Degenerate, Doped Mott Insulators

Adolfo Avella

Università degli Studi di Salerno, Salerno (Italy)

We elucidate the effects of defect disorder and e-e interaction on the spectral density of the defect states emerging in the Mott-Hubbard gap of doped transition-metal oxides, such as $Y_{1-x}Ca_xVO_3$. A soft gap of kinetic origin develops in the defect band and survives defect disorder for e-e interaction strengths comparable to the defect potential and hopping integral values above a doping dependent threshold; otherwise only a pseudogap persists. These two regimes naturally emerge in the statistical distribution of gaps among different defect realizations, which turns out to be of Weibull type. Its shape parameter k determines the exponent of the power-law dependence of the density of states at the chemical potential ($k - 1$) and hence distinguishes between the soft gap ($k \geq 2$) and the pseudogap ($k < 2$) regimes. Both k and the effective gap scale with the hopping integral and the e-e interaction in a wide doping range. The motion of doped holes is confined by the closest defect potential and the overall spin-orbital structure. Such a generic behavior leads to complex non-hydrogenlike defect states that tend to preserve the underlying C-type spin and G-type orbital order and can be detected and analyzed via scanning tunneling microscopy.

Tue 15:30 - Simone Peli

The room temperature prodrome of charge-order in copper oxides

Simone Peli

Interdisciplinary Laboratory for Advanced Material Physics (I-LAMP) and Mathematics and Physics Department,
Università Cattolica del Sacro Cuore, Brescia (Italy)

An intrinsic instability towards inhomogeneous states is emerging as the prominent feature of underdoped cuprates and manifests itself in a variety of ways including the spontaneous emergence of charge-order patterns at low temperature. The experimental evidences show a general trend where various instabilities, that break different symmetries at the nanometric scale, appear below a characteristic temperature and only up to a critical hole doping p_cr. This revives the long debated question whether this behaviour is just the consequence of the tendency to develop a specific long-range symmetry-broken phase, or it is the low-energy manifestation of a more general precursory state, which arises from strong electronic correlations suddenly changing at p_{cr}. This question is addressed by investigating the ultrafast dynamics of the O-2p→Cu-3d charge-transfer process in $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$, and by linking these results to the doping evolution of the charge-order instability on the same material. In a recent work we demonstrate that the doping p_{cr}, at which the amplitude of the spontaneous charge modulation vanishes at low temperature, also marks a sharp and drastic change in the character of the Cu-3d and O-2p wavefunctions, that turn from localized - as in a Mott insulator - to delocalized - as in a conventional metal. Since the $p=p_{cr}$ turning point is observed at room temperature, we conclude that there exists an underlying correlated state, characterized by the localization of the Cu-O wavefunctions and the related quenching of the O-2p→Cu-3d charge fluctuations, that is precursor to the low-temperature charge-order and, possibly, to the other instabilities that fan out from a zero-temperature quantum critical point at p_{cr}.

Tue 16:30 - Matteo Gatti

Coupling of excitations: correlation beyond the quasiparticle picture

Matteo Gatti[1,2,3,*]

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We discuss the fingerprints of electronic correlation in the photoemission spectroscopy of the valence band of correlated oxides.
We first illustrate the role of Fock exchange in the band structure [1] and we analyze electron hybridization properties in connection with the photon-energy dependence of the spectra [2-3].
We then focus on photoemission satellites, which are a genuine signature of electronic correlation requiring to go beyond a quasiparticle picture. We show that they can be understood in terms of the coupling between different elementary excitations, as in the case of plasmon sidebands [3-4].
We discuss how this coupling can be explained by advanced calculations based on parameter-free many-body perturbation theory that combine GW-like approximations for the self-energy with the cumulant expansion of the Green's function [5-6]. In this framework, the key physical ingredient is the dynamical screening of Coulomb interaction, containing electron-hole and plasmon excitations. It can be accurately calculated in the random-phase approximation (RPA) or by solving the Bethe-Salpeter equation [7] (including excitonic effects beyond the RPA). It can be also measured independently by loss spectroscopies, such as Electron Energy Loss Spectroscopy (EELS) or Inelastic X-ray Scattering (IXS) [8].
We therefore advocate the combination of bulk-sensitive photoemission and EELS/IXS as a powerful tool to understand the effect of the electronic interaction in correlated materials.

The presented results have been obtained in collaboration with many colleagues in the LSI Theoretical Spectroscopy Group of the Laboratoire des Solides Irradiés (http://etsf.polytechnique.fr) and in the European Theoretical Spectroscopy Facility (http://www.etsf.eu).

Tue 17:00 - Francesco Randi

Phase separation in the non-equilibrium Verwey phase transition in magnetite

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Magnetite (Fe_3O_4) is the ideal playground to study how systems displaying a first order phase transition behave out of their equilibrium state. In fact, at T_V = 123 K magnetite undergoes the so called Verwey insulator to metal phase transition [1], from a low temperature charge-ordered [2] and insulating phase to a high-temperature charge-disordered and conducting phase. The local charge-order can be destroyed through excitation with 1.5 eV light pulses and the transition can therefore be straightforwardly studied in pump-probe experiments. This possibility has been recently demonstrated in an out-of-equilibrium x-ray study [3], showing that above a threshold pump fluence the phase transition can be induced in a sample at $T<T_V$.

I will present the characterization of the out-of-equilibrium optical properties of magnetite in the visible after an excitation with 1.5 eV pump pulses [4]. Pump pulses with fluences well above the threshold for the triggering of the transition excite the system homogeneously to the high-temperature phase. Close to the threshold, instead, the variation of the reflectivity displays features that can be associated to the nucleation of the high-temperature phase and the occurrence of phase separation in the sample. These features are the non-separability of the response of the system, the spectroscopic identification of the dynamical nucleation of the conducting phase, and the close correspondence between the close-to-threshold fluence regime and the delivery of the latent heat of the transition.

Our results on phase separation in the system may have a general relevance beyond the particular case-study of magnetite. Although the details could be different, the outlined behavior may be valid in general for photo-excited out-of-equilibrium systems displaying a first order phase transition. Moreover, this picture suggests that a non-

separable dynamical response may be a general fingerprint of out-of-equilibrium phase separation and may represent a straightforward way to identify it in other out-of-equilibrium experiments.

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Tue 17:15 - Lorenzo Malavasi

Origin od colossal magnetoresistance in $LaMnO_3$ manganites

Lorenzo Malavasi

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Phase separation is a crucial ingredient of the physics ofmanganites; however, the role of mixed phases in the development of the colossal magnetoresistance (CMR) phenomenon still needs to be clarified. We present results about the realization of CMR in a single-valent $LaMnO_3$ manganite. It was found that the insulator-to-metal transition at 32 GPa is well described using the percolation theory. Pressure induces phase separation, and theCMR takes place at the percolation threshold. A large memory effect is observed together with the CMR, suggesting the presence of magnetic clusters. The phase separation scenario is well reproduced, solving a model Hamiltonian. The present results demonstrate in a clean way that phase separation is at the origin of CMR in $LaMnO_3$.

Tue 17:45 - Chiara Bigi

Electronic properties of epitaxial hole/electron doped $La_{0.7}(Ba,Ce)_{0.3}MnO_3$ thin films by photo-emission spectroscopies

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High quality epitaxial manganite thin (i.e. about 30 nm) films were grown by means of Pulsed Laser Deposition system, implanted on the operational infrastructure of the APE-NFFA laboratory [1]. Such an infrastructure provides in a suite of interconnected UHV chambers all the surface science environment and methods that will support the manipulation and characterization of the as-grown PLD samples directly connected to surface-sensitive probing technique using Elettra synchrotron facility. All the surface-related problems were therefore circumvented by allowing the synthesis and the characterization within the same UHV manifold. The dependency of the nature of charge carriers (i.e. holes and electrons) on the electronic properties of $La_{0.7}(Ba,Ce)_{0.3}MnO_3$ oxide manganite thin films has been investigated. X-ray diffraction technique were used to investigate the bulk structural properties and demonstrated the substrate/film epitaxy relation. Low-energy electron diffraction (LEED) were also employed to examine the surface structure and quality of PLD-grown manganite films, which show perfectly square and flat MnO_2 sheets. In particular, LEED images indicated that the film surfaces are of high quality and show no evidence of surface reconstruction. In order to explore the electronic properties of the grown films, X-ray photoemission spectroscopy (XPS) and angular-resolved photoemission spectroscopy (ARPES) experiments, by using synchrotron radiation, were performed on untreated in-situ transferred manganites thin films. Modification in the valence band as well as the Mn 2p photoemission spectra were observed by varying the nature of the charge carriers (i.e. holes and electrons). Recent results about the Fermi's surface features investigated by means of ARPES will be also discussed.

[1] http://www.trieste.nffa.eu/

Wed 09:00 - Gianfranco Pacchioni

Two-dimensional oxides: from microelectronics to nanocatalysis

Gianfranco Pacchioni

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Graphene is the prototype of two-dimensional materials, but is not the only one. SiO_2 films of few nanometers thickness grown on Si have been the basis of the microelectronics revolution in the second half of last century. In general, ultrathin oxide films grown on a metal, also called two-dimensional oxides, have a wide range of applications [1]. Oxides at the nanoscale may exhibit specific surface morphology, physical properties, chemical reactivity, thus providing new opportunities for the design of innovative materials. Here we will address in particular the role of two-dimensional oxides for heterogeneous catalysis. Theory has a very important role in this field and, in combination with experiments, can answer several important questions like: are the electronic properties of an oxide film of just a few atomic layers similar to those of the corresponding crystalline phases? How thick an oxide film has be to recover typical bulk properties? How important is the formation of a metal/oxide interface for the surface properties? What is the role of the strain in the supported layer? These and other related questions will be addressed in this talk by discussing transport phenomena across two-dimensional oxides (charging effects), the structural flexibility of oxide ultrathin films, nanoporosity, and in general the possibility to design nano-structured oxides with new properties and functionalities [2,3].

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Wed 09:40 - Alberto Verdini

Excess electrons distribution in TiO_2(110) and Mg:TiO_2(011) surfaces

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Titanium dioxide is a metal oxide with many relevant technological properties for photocatalysis, chemical reactivity, electrical conductivity and solar energy harvesting. TiO_2 is an inert insulator in stoichiometric form and it can be easily reduced into an n-type semiconductor TiO_{2-x} with the trasformation of Ti^{4+} to Ti^{3+} ions. This reduction is also characterized by the excess electrons populating localized Ti 3d states in the band gap [1]. These electrons can be well characterized by the presence of a defect state at about 0.8 eV below the Fermi level [2]. Moreover, in the case of very low defect content, Ti3d states can be exalted through resonant valence-band photoemission process where, at resonance, the direct photoemission of a valence-band electron interferes with the two-step autoionization process leading to the same final state. It has been measured the angular distribution and the corresponding PhotoElectron Diffraction (PED) pattern of the defect state in resonant conditions for the rutile TiO2(110) surface and mapped its distribution in the case of a non-stochiometric surface [3] and after deposition of Na on a stoichiometric surface [4]. The main finding was the demonstration that charge distribution of the band gap state is essentially an intrinsic property of the TiO_2 (110) surface, because largely independent of the way excess electrons are created. Within this framework we moved to study another rutile surface – the (011) - in the presence of Mg. Mg is a common contaminant of TiO_2 and, by thermal annealing of the sample, it is possible to make it segregate from the bulk of the sample up to the surface. Both core level and valence band photoemission experiments were performed and the spectra show a decrease of the defect state linked to Mg presence. PED patterns were also recorded in order to study the localization of magnesium in the TiO_2 surface layers. The experimental data set allows to exclude the formation of metallic Mg clusters on the surface and, rather, to point to the substitution of Mg into the Ti lattice sites. The decrease of the defect state intensity in the band gap observed in the presence

of Mg is due to the formation of MgO which takes the role of "metal oxide dopant" for the TiO_2, since doping with a metal oxide (i.e. ionic doping) does not induce electron excess.

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Wed 10:10 - Federico Cilento

Time-resolved XUV photoemission: a new clue for understanding the ultrafast dynamics in copper oxides

F. Cilento, S. Peli, A. Crepaldi, G. Manzoni, A. Sterzi, C. Cacho, E. Springate, M. Berciu, A. Damascelli, F. Parmigiani, and C. Giannetti.

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High temperature superconductivity in copper oxides is among the most intriguing phenomena concerning strongly-correlated materials. Cuprates are characterized by a complex Fermi Surface, where nodal and antinodal quasiparticles display markedly different properties and are thought to hide the key for understanding the unique properties of cuprate superconductors. Here we combine the unique momentum resolution of ARPES with a non-equilibrium approach to study the dynamics of quasiparticles over the entire Brillouin Zone of the Y-Bi2212 compound, by using an ultrafast HHG XUV photon source. For the first time, we map both the nodal and antinodal excitations, revealing a peculiar transient surplus of positive charge at the antinodes. Moreover, we study the dynamics of the Mott-like excitations involving O 2p states lying 1.5 eV below the Fermi level. In cuprates, these high-energy excitations are intertwined with the electronic properties at the Fermi level, and a challenge is to understand how the high-energy physics associated to Mott-like excitations is involved in the condensate formation. We reveal a long-lasting dynamics of the O 2p states, that is interpreted within the three-band Hubbard model where holes interact with the antiferromagnetic background. Finally, we discuss a novel approach for studying via TR-ARPES with high energy and momentum resolution and limited space charge the quasiparticle dynamics over the entire Brillouin Zone of copper-oxides, and discuss the most recent developments in the field.

Wed 10:40 - Daniele Fausti

Disclosing fluctuations of lattice atomic positions by non-equilibrium optical experiments

Daniele Fausti

Università degli Studi di Trieste, Italy

Fluctuations of the atomic positions are at the core of a large class of unusual material properties ranging from quantum para-electricity and charge density wave to, possibly, high temperature superconductivity. Their measurement in solids is subject of an intense scientific debate focused on the research of a methodology capable of establishing a direct link between the variance of the ionic displacements and experimentally measurable observables. In this presentation I will introduce our new approach to address fluctuation by means of non-equilibrium optical experiments performed in shot-noise limited regime. The variance of the time dependent atomic positions and momenta is directly mapped into the quantum fluctuations of the photon number of the scattered probing light. A fully quantum description of the non-linear interactions between photonic and phononic fields pave the way for a direct measurement of fluctuation in complex systems.

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http://arxiv.org/abs/1507.04148 (to be published in Nat. Comm.)

Wed 11:40 - Lorenzo Del Re

Non-equilibrium and non-homogeneous phenomena around a first-order quantum phase transition

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We consider non-equilibrium phenomena in a very simple model that displays a zero-temperature first-order phase transition. The quantum Ising model with four-spin exchange is adopted as a general representative of first-order quantum phase transition that belongs to the Ising universality class, such as for instance the order-disorder ferroelectric transitions, and possibly first-order T = 0 Mott transitions. The Ising model with a four spin interaction has been invoked to describe the first order paraelectric-ferroelectric phase transition, especially in order-disorder ferroelectrics[1]. Here we propose a link to another equally interesting class of first order phase transitions: the Mott metal-to-insulator transition.
Castellani, Di Castro, Feinberg and Ranninger[2] suggested that the finite temperature transition from a paramagnetic metal to a paramagnetic Mott insulator in V_2O_3 belonged to the Ising universality class. This conjecture was later put by Kotliar, Lange and Rozenberg[3] on firm theoretical grounds after the development of dynamical mean field theory (DMFT).[4] It was finally experimentally confirmed both in V_2O_3 [5] and in organic compounds.
More recently, the half-filled single-band Hubbard model on an infinitely coordinated lattice, which is the limit where DMFT is exact, was rigorously proven to be mappable onto a model of Ising spins coupled to non-interacting electrons.[6-7]
The mean-field decoupling of the Ising degree of freedom from the electronic ones leads to an effective mean-field Hamiltonian for the Ising spins that is exactly a standard infinitely-connected Ising model in a transverse field.
If we assume the above Ising dictionary to hold even when the zero-temperature Mott transition becomes first order, then we can conjecture that the Hamiltonian with four-spin exchange might provide a sensible mean-field description of that transition too.
In particular, we address quantum quenches in the exactly solvable limit of infinite connectivity and show that, within the coexistence region around the transition, the system can remain trapped in a metastable phase, so long as nucleation can be

ignored. We then study in the same model static but inhomogeneous phenomena that take place at surfaces and interfaces. The first order nature implies that both phases remain locally stable across the transition, and with that the possibility of a metastable wetting layer showing up at the surface of the stable phase, even at T = 0. We use mean-field theory plus quantum fluctuations in the harmonic approximation to study quantum surface wetting.

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Wed 11:55 - Etienne Janod

Universal out-of-equilibrium insulator to metal transitions induced by electric field in Mott insulators

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Mott insulators represent a broad class of materials that should be metallic according to conventional band theory, but are actually insulators due to on-site electron-electron repulsion. In such systems, insulator to metal transitions (IMT) can be induced at thermodynamic equilibrium by two independent tuning parameters, the electronic doping and the application of pressure.
Beside these well-established IMT mechanisms, recent developments have unveiled the possibility to trigger out-of-equilibrium IMT in Mott insulators, by applying either ultra-short laser pulses or electric fields. Researches carried out in our group have revealed a universal behavior under electric field in several families of canonical Mott insulators, [1] such as the chalcogenide compounds AM_4Q_8 (A = Ga, Ge; M = V, Nb, Ta, Mo; Q = S, Se, Te) [2] and $Ni(S,Se)_2$, the molecular compound $[Au(Et\text{-}thiazdt)_2]$ [3] and the time-honored oxide $(V_{1-x}Cr_x)_2O_3$.[4] In all these narrow gap (E_{gap}= 0.1 to 0.4 eV) Mott insulators, an abrupt drop of electrical resistance occurs above a threshold electric field E_{th} typically in the 1-10 kV/cm range. This "resistive" transition, first volatile (*i.e.* appearing only during the electric pulse application) for fields slightly above E_{th}, becomes non-volatile at larger electric fields (5 to 10 E_{th}). Moreover, the application of series of pulses allows to cycle between low and high resistance states, which allows envisioning applications in non-volatile memories and neuromorphic systems. [5] STM/STS experiments indicate that the non-volatile resistive transitions are filamentary-like and are related to a Mott insulator to metal transition at the nanoscale. [6]
Our recent study on the AM_4Q_8 family showed that the threshold fields E_{th} scale with the Mott-Hubbard gaps E_G as $E_{th} \propto E_G^{2.5}$.[7] Interestingly such a power law dependence also exists in classical semiconductors like InSb, Ge or Si : in these systems, an impact ionization leads to an electronic avalanche with a sudden drop of resistance. Our work therefore suggests that a similar mechanism may also exist in Mott insulators. Recent results related to the temperature dependence of the

threshold field E_{th}, shedding new light on the microscopic mechanism driving the volatile transition, will be presented and discussed.

* now at CIC NanoGUNE, San Sebastian (Spain)

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Wed 12:25 - Mariela Menghini

Exploring the metal-insulator transition in pure and doped V_2O_3 (ultra)thin films

Mariela Menghini

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The metal-insulator transition (MIT) in vanadium oxides is a long-standing topic of experimental and theoretical research in condensed matter physics. In particular, vanadium sesquioxide (V_2O_3), with a very rich phase diagram as a function of temperature and doping, is considered a paradigmatic example of strongly correlated materials that show an MIT.
At ambient conditions, stoichiometric V_2O_3 is a paramagnetic metal (PM) with a rhombohedral structure that is isostructural with corundum Al_2O_3. Upon cooling below 150–160 K, V_2O_3 undergoes a MIT with an increase in resistivity of over 7 orders of magnitude to an antiferromagnetic insulating (AFI) state, accompanied by a monoclinic distortion. Doping with a small percentage of Cr stabilizes a paramagnetic insulating (PI) phase at high temperature that is isostructural with respect to the PM phase. On the other hand, a small percentage of Ti doping or an oxygen excess results in a gradual decrease of the PM-AFI transition temperature down to 0K, stabilizing the PM phase at all temperatures.
In this talk I will present our results on the study of structural and electrical properties of pure and Cr-doped V_2O_3 (ultra)thin films. We observe that the MIT is strongly attenuated in films with thicknesses up to few units cells grown on Al_2O_3. However, when these extremely thin films are grown on a better lattice-matched material such as Cr_2O_3 the MIT is recovered. On the other hand, we have also studied the effects of doping the V_2O_3 films with Cr. Interestingly, we observe a collapse of the insulating state for low doping concentration (between 1% and 4%). This is likely caused by a small excess of oxygen present in the thin films.
Our findings show the importance of the effects of strain and doping on the MIT in V_2O_3. These results are not only interesting from the point of view of the physics of strongly correlated materials but can also be relevant for possible applications of MIT materials in devices.

Wed 12.55 - Michele Fabrizio

Non-Zener electric breakdown and other surprises near a first-order Mott transition

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The conventional portrait of Mott insulators overlooks that Mott transitions are mostly first order, implying an extended insulator metal coexistence. As a result, bias or light may nucleate long-lived metastable metal droplets within the stable insulator, a phenomenon that might explain recent intriguing experiments on narrow-gap Mott insulators. In this talk I will show how this expectation is realized in a very simple model that has a quite wide coexistence region and might be representative of a large class of Mott insulators with a d-d charge-gap rather than a direct gap between lower and upper Hubbard bands. In particular I will show that the electric breakdown induced by an external bias is different from the Zener's breakdown of conventional semiconductor. I will also mention other intriguing