**Addressing the Origin of Conductivity in Two-dimensional Electron Gases at Oxide Interfaces.**

Fabio Miletto Granozio
CNR-SPIN UOS Napoli, Complesso Universitario di Monte Sant’Angelo, Via Cintia, IT-80126 Napoli

Oxide interfaces exhibit sometimes functionalities absent in both the constituent materials. A prototypical example of this emergent behaviour is provided by the 2-dimensional electron gas first found at LaAlO₃/SrTiO₃ interfaces. In this work, the properties of the 2DEGs found at the LaAlO₃/SrTiO₃, LaGaO₃/SrTiO₃, NdGaO₃/SrTiO₃ and Al₂O₃/SrTiO₃ interfaces are addressed and compared. Interfaces based on the respective amorphous counterparts, also showing a highly mobile electron gas, are also investigated. Specific experiments aimed at highlighting similarities and differences in the two systems were performed. Our results are in agreement with an electrostatic mechanism being responsible for the conductivity of crystalline interfaces.

**Spectroscopy Views of Low Dimensional Electron Gas (LDEGs) at STO Surface and LAO/STO Interface: Final Depiction**

Milan Radovic, Paul Scherrer Institut, 5232 Villigen PSI

The interfaces between transition metal oxides show astonishing properties: tunable insulator-superconductor-metal transitions, large magnetoresistance, coexisting nano-domains of ferromagnetism and superconductivity, etc. More recently, LDEGs was discovered also at the (001) surface of SrTiO₃ (STO) single crystals. Therefore, a complete understanding of the LDEGs becomes a basic step for a clear interpretation of the electronic properties of interfaces obtained by combining STO and other oxides. Here we show, using and angle-resolved photoemission spectroscopy (ARPES) and spin-angle-resolved photoemission spectroscopy (SARPES) and Resonant Inelastic X ray scattering (RIXS), complete picture of the LDEGs electronic structure at STO surface and LAO/STO interface.

**Large Rashba induced modulation of the Shubnikov-de Haas oscillations at the LaAlO₃-SrTiO₃ interface.**

Alexandre Fête ¹, Stefano Gariglio ¹, Christophe Berthod ¹, Danfeng Li ¹, Daniela Stornaiuolo ¹, Marc Gabay ², Jean-Marc Triscone ¹

¹ Département de Physique de la Matière Condensée, University of Geneva
24, Quai Ernest-Ansermet, 1211 Geneva
² Laboratoire de Physique des Solides, Université Paris-Sud, FR-91405 Orsay

In this work, we study the Fermi surface of the conducting LaAlO₃/SrTiO₃ interface [1] using Shubnikov-de-Haas (SdH) oscillations. We show that a scenario consisting of a single Rashba spin(-orbit) split band best describes our data [2-4]. Interestingly, we observe that the Rashba splitting is of the same order of magnitude than the Fermi energy of the oscillating carriers, revealing a rather unconventional regime realized at this interface. Studying the gate voltage tuning of the SdH oscillations, we put into evidence sharp deviations in the Landau levels evolution as a function of magnetic field and doping, that suggest physics beyond the independent particle approximation.

Quenched Magnon dispersion by oxygen sub-lattice reconstruction in SrCuO₂ thin films

Marcus Dantz 1, Valentina Bisogni 1, Jonathan Pelliciari 1, Yaobo Huang 1, Paul Olalde-Velasco 1, Debakanta Samal 2, Gertjan Koster 2, Thorsten Schmitt 1
1 Paul Scherrer Institut, 5232 Villigen
2 University Twente, Faculty of Science & Technology, Carre, 3215, NL-7500 Enschede

Multi-layered thin films of cuprates allow studying how the crystal field and the dispersion of magnetic excitations can be sensitively modified.[1][2] In (SrCuO₂)n/(SrTiO₂)2 superlattices, in particular, a structural transformation from bulk planar to a pyramidal local environment has recently been observed that is driving an orbital reconstruction for n<5.[3] Here we present results regarding the influence of this orbital reconstruction on the magnetic dispersion using resonant inelastic x-ray scattering at the Cu L₃ edge. A clear quenching of the magnon dispersion for SrCuO₂ layer thicknesses of 3 unit cells is observed.


(S-)ARPES investigation on the electronic and spin structures of strongly correlated system SmB₆ and experimental realization of the first topological Kondo insulator

Nan Xu 1, Pabitra Biswas 1, Jan Hugo Dil 2, Rajendra Dhaka 1, Gabriel Landolt 3, Stefan Muff 2, Christian Matt 1, Xun Shi 1, Nicholas Plumb 1, Milan Radovic 1, Ekaterina Pomjakushina 1, Kazimierz Conder 1, Alex Amato 1, Sergey Borisenko 4, Rui Yu 5, Hongming Weng 5, Zhong Fang 5, Xi Dai 5, Joël Mésot 1, Hong Ding 5, Ming Shi 7
1 Paul Scherrer Institut, 5232 Villigen PSI
2 EPFL, 1015 Lausanne
3 Physik-Institut, Universität Zürich, Winterthurerstr. 190, 8057 Zürich
4 Institute for Solid State Research, IFW Dresden, DE-01171 Dresden
5 Beijing National Lab. for Condensed Matter Physics and Institute of Physic, CN-100190 Beijing

Our ARPES study revealed that the surface states reside within the Kondo band gap in SmB₆, and form three Fermi surfaces in the first surface BZ. The odd number of surface bands crossing the Fermi level fulfills the necessary condition of topological states, and in good agreement with theoretical calculations. Using spin-resolved ARPES, we investigated the spin texture of the surface states. The surface states are spin polarised locking with momentum. The spin-helical structure fulfills the requirement of time-reversal symmetry and the crystal symmetry. Our results indicate SmB₆ is the first realisation of the topological Kondo insulator.

A two-dimensional electron gas at the (111) surface of SrTiO₃

Siobhan McKeown Walker 1, Alberto De La Torre 1, Anna Tamai 1, Phil King 2, Saeed Bahramy 3, Felix Baumberger 1
1 DPMC, Université de Genève, 24 Quai Ernest-Ansermet, 1211 Geneva
2 SUPA, University of St Andrews, North Haugh, St Andrews KY16 9SS, UK
3 RIKEN, Center for Emergent Matter Science, 304-1/301/204 Frontier Research Lab., Wako, Japan

Two-dimensional electron gases (2DEGs) at surfaces or interfaces of SrTiO₃(100) emerged as model systems for studying the physics of all-oxide electronic devices. Here, we report the direct spectroscopic observation of quasi two-dimensional electronic states with carrier densities up to 2·10¹⁴ cm⁻² on the surface of single crystal SrTiO₃(111). Our ARPES data show a shallow bandwidth and anisotropic, six-fold symmetric Fermi surface with effective masses different from the bulk. The 2DEG is inert to details of the surface condition and can be reversibly depleted and created by exposure to atomic oxygen and UV radiation. This raises new prospects of tuning surface and interface states with properties not realized by bulk doping.
The spectroscopic power of SX-ARPES arises by virtue of merging the enhanced probing depth, accurate 3D momentum resolution and resonant photoexcitation allowing elemental and chemical state specificity (Strocov et al, Synchr. Rad. News 27, N2, 31 (2014)). The advanced SX-ARPES instrumentation at the Swiss Light Source has allowed stretching this technique from the traditional applications to 3D bulk crystals towards most photon-hungry cases of buried systems. We overview this recent development vector with a few characteristic cases, including 3D strongly correlated transition metal oxides (magnanites La$_{1-x}$Sr$_x$MnO$_3$ with their colossal magnetoresistance), buried interfaces (quantum-well states at the LaAlO$_3$/SrTiO$_3$ interface) and impurity systems (ferromagnetic Mn impurity band in the diluted semiconductor GaMnAs).

Watching optically excited electrons decay in graphene

Jens Christian Johanssen, Marco Grioni
Institut de physique de la matière condensée, EPFL, Station 3, 1015 Lausanne

Exploiting the unique properties of graphene in future optoelectronic devices inevitably involves the generation of hot electrons. We have carried out the first direct study of the ultrafast hot electron dynamics in graphene with time- and angle-resolved photoemission. Here, we will present the results of this study that demonstrates a quasi-instant thermalization of the electrons to a temperature of 2000 K and a disentanglement of the subsequent decay into excitations of optical and acoustic phonons via supercollisions. The possibility of carrier multiplication will also be addressed. This process could play an important role in the realization of efficient photovoltaic devices.

Deposition of molybdenum nitride by magnetron sputtering

Laurent Marot, Elcin Külah, Roland Steiner, Lucas Moser, Ernst Meyer
Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel

Molybdenum nitride films have been prepared by magnetron sputtering for several experimental conditions. The films were characterized by in-situ XPS (X-ray photoelectron spectroscopy), UPS (ultraviolet photoelectron spectroscopy), XRD and SEM. The effects of deposition parameters on the resulting crystallite structure and surface roughness, and hence on the reflectivity, were investigated. A low oxygen atomic concentration (< 5%) was achieved using a liquid nitrogen cold trap system and without breaking the vacuum by XPS measurements, the binding between Mo and N were characterized for specific phases, i.e. MoN and Mo$_2$N. So we have no oxide compared to previous studies.

Tuning Molecular Orbitals of Manganese Phthalocyanine on h-BN/Rh(111) Nanomesh

Liwei Liu, Roland Widmer, Thomas Dienel, Oliver Gröning, EMPA, Überlandstrasse 129, 8600 Dübendorf

The electronic structure of Manganese Phthalocyanine (MnPc) molecules on Boron nitride grown on Rh(111) surface (nanomesh) were studied by low-temperature Scanning Tunneling Microscopy (STM). The MnPc molecules are trapped by the pores of the nanomesh, revealing the template effect of substrate. The molecules can be divided into three categories which show very different bias-dependent-topography, where different categories of molecules can be reversibly switched to each other. The switching is induced by the STM. We attribute the difference to the exact adsorption configuration of the molecules. Our results give insights on how the electronic properties of the adsorbates are tuned by a surface supported ultra-thin insulator.
Electronic Decoupling of Molecular Nanostructures by Intercalating Thin Oxide Films

Okan Deniz, Carlos Sánchez, Roland Widmer, Roman Fasel, Pascal Ruffieux

EMPA, Überlandstrasse 129, 8600 Dübendorf

Covalently bonded molecules/systems (CBS) have attracted significant interest due to their capability of utilization in modern devices. However, their electronic properties couldn’t be precisely investigated because of the metal substrate that is needed as catalyst for CBS fabrication. Few approaches to circumvent this limitation are; transferring molecules onto an insulating substrate or, intercalating thin insulator film \[1\] to electronically decouple CBS from substrate. In-situ intercalation of thin insulator films allows well-defined metal/insulator interfaces and the direct application of surface science techniques such as XPS, STM, STS and LEED. We focus on Au(111)/SiO\textsubscript{x} system’s structure and interface. The first results of decoupling of CBS will be discussed.

\[1\] Nano Lett. 12,4503

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Inspecting the impact of epitaxial strain on nickelate thin films.

Sara Catalano 1, Marta Gibert 1, Valentina Bisogni 2, Oleg Peil 1, Michel Viret 1, Ronnie Sutarto 3, Feizhou He 3, Pavlo Zubko 4, Raoul Scherwitzl 1, Claudio Mazzoli 5, George A. Sawatzky 6, Antoine Georges 1, Thorsten Schmitt 7, Jean Marc Triscone 1

1 Dép. de Physique de la Matière condensée, Université de Genève, quai Ernest-Ansermet 24, 1211 Genève
2 Brookhaven National Laboratory, 75 Brookhaven Avenue, Bldg. 725B Upton, New York, USA
3 Canadian Light Source Inc., 44 Innovation Boulevard, Saskatoon, Canada
4 London Centre for Nanotechnology, 17-19 Gordon Street London, UK
5 Politecnico di Milano, Piazza Leonardo da Vinci 32, IT-20133 Milano
6 Department of Physics and Astronomy, University of British Columbia, 2329 West Mall, Vancouver, Canada
7 Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI

Perovskite nickelates (R-NiO\textsubscript{3}, R=Rare Earth) exhibit a metal to insulator transition (MIT), whose temperature (T\textsubscript{MI}) changes in the range 600-0 K as the R volume increases. These compounds also undergo a paramagnetic to antiferromagnetic (Néel) transition, with T\textsubscript{Néel}=T\textsubscript{MI} for R=Sm, or T\textsubscript{Néel}<T\textsubscript{MI} for R\textless;Sm. Here, we investigate thin films of SmNiO\textsubscript{3} and NdNiO\textsubscript{3}, finely tuning their lattice parameters through epitaxial strain. Transport and Resonant Soft X-ray Diffraction measurements reveal a dramatic impact of such structural changes on T\textsubscript{MI} and T\textsubscript{Néel}. Through Density Functional Theory, we clarify the role played by strain in modifying the band structure of these systems.

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Picking out a Single layer of a Metal-Supported Ultrathin Oxide Film using Resonant Auger Spectroscopy

Thomas Jaouen 1, Clément Didiot 1, Elia Razzoli 1, Gaël Monney 1, Baptiste Hildebrand 1, Matthias Muntwiler 2, Philipp Aebi 1

1 Département de Physique, Université de Fribourg, Chemin du Musée 3, 1700 Fribourg
2 Swiss Light Source, Paul Scherrer Institute, 5232 Villigen PSI

By combining x-ray excited Auger electron diffraction experiments and multiple scattering calculations we first reveal a layer-resolved shift for the Mg KLL Auger transition in MgO ultrathin films on Ag(001). Next, we focus on the influence of the solid state environment on the threshold Auger process by observing the KLL Auger decay while scanning the photon energy through the Mg K-edge (PEARL endstation). We show that the K core excitation in interface, surface, and bulk unoccupied states leads to separate features in the Mg K pre-edge which gives access to unique fingerprints in the KLL Auger decay.

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Tuning of the depolarization field and nanodomain structure in ferroelectric thin films

Céline Lichtensteiger 1, Stéphanie Fernandez-Pena 1, Christian Weymann 1, Pavlo Zubko 2, Jean-Marc Triscone 1

1 DPMC - University of Geneva, 24 Quai Ernest Ansermet, 1211 Geneva
2 London Centre for Nanotechnology and Department of Physics and Astronomy, 17-19 Gordon Street, London, UK

In ferroelectric ultrathin films, the depolarization field arising from uncompensated surface bound charges will dramatically alter the properties of an ultrathin film. Using piezo-force microscopy, we investigate the intrinsic nanodomain structure of PbTiO\textsubscript{3} ultrathin films. By changing the degree of screening, the domain structure can be modified or even suppressed in favour of a uniform monodomain state. The polarization stability after switching has also been studied as a function of the depolarization field. Additionally, reducing the PbTiO\textsubscript{3} thickness leads to a change in the size and shape of the domains, which transform from large nanodots to narrow stripes.
277 Superconducting Interfaces between Artificially-Grown LaAlO$_3$ and SrTiO$_3$ Thin Films

Danfeng Li, Stefano Gariglio, Claudia Cancellieri, Wei Liu, Alexandre Fete, Daniela Stornaiuolo, Jean-Marc Triscone, University of Geneva, 24 quai Ernest-Ansermet, 1211 Geneva

We present for the first time the successful realization of a superconducting 2DEG at interfaces between artificially-grown LaAlO$_3$ and SrTiO$_3$ thin films. Our results highlight the importance of two factors - the growth temperature and the SrTiO$_3$ termination. By adopting an extremely high SrTiO$_3$ growth temperature, we demonstrate a way to realize metallic, down to the lowest temperature, and superconducting 2DEG at interfaces between LaAlO$_3$ layers and artificially-grown SrTiO$_3$ thin films. This study paves the way to the realization of functional LaAlO$_3$/SrTiO$_3$ multilayers and we also demonstrate the interesting superconducting properties of these LaAlO$_3$/SrTiO$_3$ multilayers.

278 Mott- to wide-band insulator transition of LaTiO$_3$/LaAlO$_3$ heterostructures revealed by XAS and RIXS

Jonathan Pelliciari 2, Valentina Bisogni 1, Milan Radovic 2, Marco Salluzzo 3, Yaobo Huang 1, Paul Olalde-Velasco 1, Zoran Ristic 1, Nicholas Plumb 1, Luc Patthey 1, Joël Mésot 1, Thorsten Schmitt 1
1 Brookhaven National Lab, BNL, 11973 Upton, USA
2 Paul Scherrer Institute, 5232 Villigen PSI
3 CNR-SPIN, Complesso Monte Santangelo Via Cinthia, IT-80126 Napoli

Advances in thin film deposition techniques enable to create thin films of oxides heterostructures. One of the most important systems, LaAlO$_3$/SrTiO$_3$ heterostructures, hosts a 2D conductive layer at the interface between wide-band insulators. Superlattices composed of LaAlO$_3$ (band-insulator) and LaTiO$_3$ (Mott-insulator) present instead an increasing insulating behavior when reducing the LaTiO$_3$ thickness from 10 u.c. to 2 u.c. X-ray absorption (XAS) and Resonant Inelastic X-ray Scattering (RIXS) of this system show evidence of a change in the Ti ground state configuration from the nominal Ti$^{3+}$ (10 u.c.) to an almost pure Ti$^{4+}$ (2 u.c.). These results suggest a transition from a Mott- to a wide-band insulator.

279 Influence of oxygen plasma treatment on the electronic structure and photo-electrochemical properties of iron oxide films for solar water splitting photoanodes

Yelin Hu 1, Florent Boudoire 1, Iris Hermann-Geppert 2, Peter Bogdanoff 3, Giuseppino Fortunato 4,
Bongjin Simon Mun 5, Giuseppino Fortunato 4, Peter Bogdanoff 3, Giuseppino Fortunato 4,
Bongjin Simon Mun 5, Giuseppino Fortunato 4
1 Laboratory for High Performance Ceramics, EMPA, Überlandstrasse 129, 8600 Dübendorf
2 Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, DE-14109 Berlin
3 Physikalisches Institut, Experimentelle Physik III, Universität Würzburg, Am Hubland, DE-97074 Würzburg
4 Tomsk State University, RU-634050 Tomsk
5 Donostia International Physics Center, UPV/EHU, ES-20080 San Sebastian

Hematite is a promising anode material for photoelectrochemical (PEC) water splitting due to its suitable chemical and physical properties. Although considerable effort has been devoted, the detailed mechanisms are still unclear. In our work, nanostructured hematite films were made by low cost dip coating procedure and its photoelectrochemical property was affected dramatically after oxygen plasma post treatment. XPS and valence band PES measurements of the hematite samples revealed a variation of structural defects (oxygen vacancies) on hematite surface as a function of plasma treating period, which matches both variations of photo-current density and of surface states investigated by impedance spectroscopy. These demonstrate strong correlation among surface state, defects and performance.

280 Spin texture of Bi$_2$Se$_3$ thin films in the quantum tunneling limit

Gabriel Landolt 2, Hugo Dil 1, Jürg Osterwalder 2, Stefan Schreyeck 3, Laurens Molenkamp 3,
Sergey Ereemeev 4, Evgueni Chulkov 5
1 Institute of condensed matter physics, EPFL, Station 3, 1015 Lausanne
2 Physik Institut, University of Zürich, Winterthurerstrasse 190, 8057 Zürich
3 Physikalisches Institut, Experimentelle Physik III, Universität Würzburg, Am Hubland, DE-97074 Würzburg
4 Tomsk State University, RU-634050 Tomsk
5 Donostia International Physics Center, UPV/EHU, ES-20080 San Sebastian

By means of spin- and angle-resolved photoelectron spectroscopy we studied the spin structure of high-quality thin films of the topological insulator Bi$_2$Se$_3$. For thicknesses below six quintuple layers the spin-polarized metallic topological surface states interact with each other via quantum tunneling and a gap opens up in the Dirac cone. Our measurements show that the resulting surface states can be described by massive Dirac
cones which are split in a Rashba-like manner due to the substrate induced inversion asymmetry. The inner and the outer Rashba branches have distinct localization in the top and the bottom part of the film.

281 Revealing the electronic ground state of ReNiO$_3$ combining high-resolution Ni-L$_3$ X-ray absorption and resonant inelastic x-ray scattering

Yaobo Huang $^4$, Valentina Bisogni $^1$, Sara Catalano $^2$, Marta Gibert $^3$, Robert Green $^3$, Raoul Scherwitzl $^2$, Shadi Balandesh $^3$, Vladimir Strocov $^4$, Pavlo Zubko $^5$, George Sawatzky $^3$, Jean-Marc Triscone $^2$, Thorsten Schmitt $^4$

$^1$ Brookhaven National Lab, BNL, 11973 Upton, USA
$^2$ Université de Genève, 24 Quai Ernest Ansermet, 1211 Geneva
$^3$ University of British Columbia, 2329 W Mall, Vancouver, Canada
$^4$ Paul Scherrer Institute, 5232 Villigen PSI

Perovskite rare-earth (Re) nickelates ReNiO$_3$ continue to attract a lot of interest thanks to their intriguing properties like sharp metal to insulator transition (MIT), unusual magnetic order and expected superconductivity. Full understanding of these materials, however, is hampered by the difficulties in describing their electronic ground state (GS). Taking a NdNiO$_3$ thin film as a representative example, we reveal with x-ray absorption (XAS) and resonant inelastic x-ray scattering (RIXS) an electronic GS configuration composed of delocalized and localized components. Our study conveys that a 3d8L-like configuration takes on the leading role in the GS of ReNiO$_3$, as proposed by recent model theories.

282 Switching of the binding motif in terpyridyne assemblies as a pathway towards distinctly different porous on-surface architectures

Thomas Nijs $^1$, Shadi Fatayer $^1$, Aneliia Shchyrba $^1$, Sylwia Nowakowska $^1$, Frederik J. Malzner $^1$, Maximilian Y. Klein $^2$, Srboljub Vujovic $^2$, Thomas A. Jung $^3$, Catherine E. Housecroft $^2$, Edwin C. Constable $^2$

$^1$ Departement Physik, Universität Basel, Klingelbergstrasse 82, 4056 Basel
$^2$ Departement Chemie, Universität Basel, Spitalstrasse 51, 4056 Basel
$^3$ Laboratory for Micro- and Nanotechnology, Paul Scherrer Institute, 5232 Villigen PSI

We present a study on the self-organization of a 4,2’:6’,4’’-terpyridine derivative, namely 4’-(1H-imidazol-4-yl)-4,2’:6’,4’’-terpyridine on Au(111) and Cu(111) single crystal. In contrast to the well-established chelating 2,2’:6’,2’’-terpyridines, this molecule includes inherent design features facilitating metal-coordination through N atoms. By combining Scanning Tunneling Microscopy (STM) and X-ray Photoelectron Spectroscopy (XPS) we are able to analyze the transition of the inter-molecular bond from hydrogen-bonding to Cu-coordination. After deposition on either Au(111) or Cu(111), two asymmetric molecules form a dimer which compensates the irregular symmetry of the building blocks and enables the formation of a 6-fold nanoporous hydrogen-bonded network. By supply of Cu adatoms to this assembly, the intermolecular binding motive changes from hydrogen bonded to metal-coordinated. Due to the increased substrate-absorbate interaction, on Au(111) the molecules were found to assemble into chains of linked heterocyclic macrocycles, which generally follow the fcc domains of the Au(111)(22x√3) reconstruction. On Cu(111) the molecules form an assembly of repeating uniform double rows.

283 Porphyrin metalation providing an example of a redox reaction facilitated by a surface reconstruction.

Gitika Srivastava $^1$, Jan Nowakowski $^{1,2}$, Christian Wäckerlin $^1$, Jan Girovsky $^{1,2}$, Dorota Siewert $^1$, Thomas Jung $^{1,2}$, Nirmalya Ballav $^3$

$^1$ Laboratory for Micro and Nanotechnology, Paul Scherrer Institute, 5232 Villigen PSI
$^2$ Swiss Nanoscience Institute, Department of Physics, University of Basel
$^3$ Department of Chemistry, Indian Institute of Science Education and Research, Mendeleev block, Pashan, IN-411008 Pune

Recently, on-surface redox chemistry [1] has received significant attention. The here discussed metalation of free-base porphyrins on surfaces provides an interesting example [2]. Metalation can be realized in different ways, one of which is on-surface self-metalation, i.e. by the reaction of free-base porphyrins with atoms released from the substrate. By employing X-Ray Photoelectron Spectroscopy and Scanning Tunneling Microscopy methods we show that the temperature at which this form of self-metalation occurs is lowered from 450 K on native to 285 K on oxygen-reconstructed Cu(001) surfaces [3].