O 90: Electronic structure III

Time: Thursday 17:15–19:30 Location: WIL C107

O 90.1 Thu 17:15 WIL C107

Implementation of PAW method in localized-basis-set SIESTA code — •Tristana Sondon and Chu Chun Fu — SRMP - CEA - Saclay, 91191 Gif-sur-yvette Cedex, France

The Projector Augmented Wave Method (PAW)has been demonstrated to be a particularly efficient and accurate approach to perform electronic structure calculations. The main advantage of this method is that it has a computational cost similar to that of a pseudo-potential calculation while retaining the key physics of all electron methods, including the correct nodal behavior of the valence electron wave functions. The SIESTA code is an efficient DFT code that uses a linear combination of pseudo-atomic orbitals (LCAO) as a basis set, and in the present form of the code, the calculations are made within the formalism of Norm-Conserving Pseudo-Potentials of the Troullier-Martins type in their fully non-local form. The PAW method is already implemented in many plane-wave codes, by modifiying the previous available Ultra-Soft pseudo-potential scheme, but in our case, more significant changes to the code are required. The inclusion of PAW is expected to achieve a combination of the high accuracy of the PAW method with a more efficient LCAO basis set. The specific characteristics and main approximations of this implementation will be reported. In order to highlight the performance of PAW, we will show detailed comparison of point defects properties in Fe and Fe-Cr alloys predicted by various pseudo-potential aproaches, with the ones calculated with the PAW method for different type of basis sets (plane-waves and LCAO).

O 90.2 Thu 17:30 WIL C107

Bulk States Confinement as a Long Range Sensor for Impurities and a Quantum Information Transfer Channel — •Pavel Ignatiev, Oleg Brovko, and Valeriy Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

We show that confinement of bulk electrons can be observed at low-dimensional surface structures and can serve as a long range sensor for the magnetism and electronic properties of single impurities or as a quantum information transfer channel with large coherence lengths. Our ab-initio calculations reveal oscillations of electron density in magnetic chains on metallic surfaces and help to unambiguously identify the electrons involved as bulk electrons. We furthermore discuss a possibility to utilize bulk states confinement to transfer quantum information, encoded in an atom's species or spin, across distances of several nanometers with high efficiency.

O 90.3 Thu 17:45 WIL C107

Work-Function Modification beyond Pinning: When Do Molecular Dipoles Count? — •Oliver T. Hofmann, David A. Egger, Gerold M. Rangger, and Egbert Zojer — Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

Control over the work function (Φ) of metals can be exerted by creating a sheet of dipoles above the surface, e.g., via depositing strong electron donors or acceptors onto the surface. For systems with strong charge-transfer character, one observes pinning of the Fermi level at the molecular level that donates or accepts electrons; i.e., Φ of the combined system is almost independent on the underlying metal and only governed by properties of the adsorbate. At the same time, molecules with intrinsic dipoles are also well known to also modify Φ. This raises the question how these effects interfere in systems inducing charge transfer and simultaneously bearing a dipole. Using density functional theory, we find [1] that intrinsic molecular dipole moments are compensated by adjustments in the amount of the charge transferred, as long as they are located spatially between the metal and the region of the pinning level of the organic molecule. In this case, the intrinsic dipoles are essentially inconsequential for the net work function. In contrast, dipole moments located outside the immediate metal/molecule junction region leave the charge-transfer unscathed. Clever design of the molecules, therefore, allows going beyond Fermi level*pinning. Along these lines, we suggest strategies for work-function changes of unprecedented magnitude. [1] Hofmann et al.,Nano Lett.,2010,10(11),pp4369

O 90.4 Thu 18:00 WIL C107

From Molecule to Monolayer: Self-Induced Quantum-Confined Stark effect in Monolayers of Polar Molecules — •Ferdinand Rissner[1], David A. Egger[1], Amir Natan[2], Thomas Körzdörfer[3], Stephan Kümmel[3], Leeor Kronik[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, TU Graz, Graz, Austria — [2]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth, Israel — [3]Physikalisches Institut, Universität Bayreuth, Bayreuth, Germany

Using density functional theory calculations, the electronic structure of the polar molecule terpyrimidinethiol is investigated in gas phase and in a 2D-periodic self-assembled monolayer (SAM). We find that hybrid functionals give qualitatively different results compared to a (semi-)-local description and rationalize this finding in terms of an orbital-dependent self-interaction error.

Upon self-assembly, we observe orbital energy shifts depending on the spatial structure of the orbital, which can render the ordering of the states a function of the SAM packing density. Related to this, the energy gap is modified and the symmetry of the frontier orbitals can change. Occupied and unoccupied frontier orbitals localize on opposite sides of the monolayer as known from the quantum-confined Stark effect. All this is caused by the internal electric field originating from the molecular dipole moments.

O 90.5 Thu 18:15 WIL C107

Local Electronic Structure and Surface Potential of Atomic Chains on Si(111)5x2-Au — •Ingo Barke, Stefan Polei, Kristian Sell, Viola von Oeynhausen, and Karl-Heinz Meiwes-Broer — Universität Rostock , Institut für Physik, Universitätsplatz 3, D-18051 Rostock

Quasi one-dimensional surface reconstructions are formed by various metals adsorbed on flat or vicinal Si(111). On Si(111)5x2-Au the spatially resolved density of states is measured by scanning tunneling spectroscopy. Spectral features are assigned to particular structural elements based on a recently proposed model [1]. In this contribution two key elements are discussed: (1) the Si honeycomb chain channel (HCC) with locally graphitic structure which is found on many chain systems, and (2) Si adatoms with an average coverage of 0.25 atom per 5x2 unit cell leading to pronounced bright protrusions in STM images. While the latter result in local electron doping, the HCC give rise to a pronounced corrugation of the surface potential perpendicular to the chains. These variations manifest themselves in energy modulations of unoccupied, image-state derived electron states.

[1] S. C. Erwin, I. Barke, and F. J. Himpsel, Phys. Rev. B 80, 155409 (2009).

O 90.6 Thu 18:30 WIL C107

Modification of field emission resonances by Cu and Cu/Ag islands on Ag(100) — •Christopher Zaum and Karina Morgenstern — Institut für Festkörperphysik, Abteilung ATMOS, Gottfried Wilhelm Leibniz Universität, Appelstr. 2, D-30167 Hannover, Germany

We deposited Cu islands containing 10 to 500 atoms on a clean Ag(100) surface at room temperature and investigated their electronic structure by STS spectroscopy with a low temperature scanning tunneling microscope. Islands containing less than 50 atoms per islands are pure Cu islands, while islands at sizes above 80 atoms per island are Cu/Ag alloy islands. STS measurements reveal that these two island types have a different impact on the field emission resonances (FERs) of the Ag(100) surface. While the observed modifications for large islands are marginal, noticeable shifts of the FERs occur for small islands. These different results in STS spectroscopy are discussed with respect to the different work functions of pure and alloyed islands. Such STS measurements could therefore be used to determine the composition of surface alloys with high spatial resolution.

O 90.7 Thu 18:45 WIL C107

Influence of Shake-Up Behaviour at Titanium Nitride Interfaces using AR-XPS — •Dominik Jaeger[1], Jörg Patscheider[1], and László Forró[2] — [1]Empa Dübendorf. Switzerland — [2]EPFL, IPMC/SB, Switzerland

Nanocomposites that consist of nanometric titanium nitride grains surrounded by an amorphous silicon nitride tissue phase, exhibit extraordinary properties such as hardness and high oxidation resistance. They originate from the interplay of grain size, nature of the tissue phase and the interface strength. In the ample literature on those nanocomposites an experimental description of their interface is largely missing. This study presents investigations on the interfaces of TiN in contact with different overlayers. Two dimensional layer system is used to probe the interfaces. Different overlayers are deposited on oxygen-free TiN by Unbalanced Magnetron Sputtering. These interfaces are investigated by Angle Resolved X-ray Photoelectron Spectroscopy (AR-XPS). To prevent contaminations at the interfaces, the samples have been transferred in situ between deposition and analysis. XPS spectra show for TiN a shake-up feature caused by extra-atomic relaxation processes. During this process electrons from the inner Ti2p shell are loosing energy due to inelastic scattering at higher occupied shells. This energy loss has been recorded for interfaces between TiN and Si3N4, Si, and AlN as overlayers. The shake-up intensities and energies provide information on the electronic states in the surrounding neighbourhood and thereby on the interfaces. The results will be discussed in terms of polarisation effects at these interfaces.

O 90.8 Thu 19:00 WIL C107

The role of diffraction in (e,2e) experiments — •Frank O. Schumann, Zheng Wei, Rajendra Dhaka, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

We have performed an electron pair emission study from a Cu(100) surface excited by a primary electron beam covering the energy range 19-100 eV. In the sum energy spectra of coincident pairs we are able to identify distributions from the *d* states and the *sp* states. We notice a strong dependence of the relative contribution of these two spectral ranges as a function of the primary energy. The curve describing this behavior resembles the LEED I-V curve of the (0,0) beam. Extending the kinematical picture for the emergence of intensity peaks in LEED to electron pairs predicts intensity maxima in fair agreement with the experimental findings. Further, we studied the pair intensity as a function of the azimuthal orientation of the sample. From simple symmetry considerations we expect a variation of the coincidence intensity. We find an asymmetry up to 20 % when we compare sum energy spectra obtained along two different main symmetry directions. We are able to make contact to selection rules obtained for a (e,2e) process and identify the valence states involved. These results are a critical test of the validity of approximations made in the theoretical description.

O 90.9 Thu 19:15 WIL C107

Double photoemission illuminates the Auger process — •Zheng Wei, Grant van Riessen, Rajendra S. Dhaka, Carsten Winkler, Frank O. Schumann, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

We performed a double photoemission (DPE) experiment on a Cu(001) surface at the BESSY-II storage ring. The energy of the linearly polarized photons was tuned to 125 eV. We are able to map out the photoelectron and Auger electron simultaneously in large energy space of 30 eV×30 eV [1]. Electron pairs emitted directly from the valence band are known to share continuously the available energy due to the fact that this process proceeds in a single-step [2]. Usually the emergence of an Auger electron is explained via a two-step process in which the relaxation leading to the Auger emission is preceded by the emission of a photo-electron. Our observation of a continuous energy sharing in the DPE intensity involving core electrons can only be explained within a single-step process.

[1] G. van Riessen, Z. Wei, R. S. Dhaka, C. Winkler, F. O. Schumann and J. Kirschner, J. Phys.:Condens. Matter **22**, 092201 (2010).
[2] F. O. Schumann, C. Winkler, J. Kirschner, Physica Status Solidi B **246**, 1483 (2009).