O 7: Surface Dynamics I

Time: Monday 11:15–13:00 Location: WIL C107

O 7.1 Mon 11:15 WIL C107

Observation of the Surface Segregation of Cu in Pd by Time-Dependend Positron-Annihilation-Induced Auger Electron Spectroscopy — •Christoph Hugenschmidt, Jakob Mayer, and Klaus Schreckenbach — FRM II und Lehrstuhl E21 Physik Department, Technische Universität München, 85747 Garching

Density functional theory calculations predict the surface segregation of Cu in the second atomic layer Pd which was not unambiguously confirmed experimentally so far. We report measurements on Pd surfaces covered with three and six monolayers of Cu using the element selective positron annihilation induced Auger electron spectroscopy (PAES) which is sensitive to the topmost atomic layer. Moreover, time resolved PAES, which was applied for the first time, enables the investigation of the dynamics of surface atoms and hence the observation of the segregation process. The time constant for segregation was experimentally determined to 1.38(0.21)h, and the final segregated configuration was found to be consistent with calculations. Within this work, we demonstrate that time dependent PAES is a novel element selective technique applicable for numerous systems for the investigation of e.g. heterogeneous catalysis, corrosion or surface alloying.

O 7.2 Mon 11:30 WIL C107

LEEM study of segregation and diffusion of impurities at Fe polycrystal surfaces — •Benjamin Borkenhagen[1], Thorsten Franz[2], Gerhard Lilienkamp[1], and Winfried Daum[1] — [1]IEPT, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]ELMITEC GmbH, Albrecht-von-Grodeck-Str. 3, 38678 Clausthal-Zellerfeld

Surface properties of applied materials are frequently related to microstructural properties such as texture, grain boundaries and stacking faults in polycrystals. The application of methods providing information on surface crystallography and topography with sub-grain lateral resolution is a most promising route for the surface characterization of such materials. Recently we have demonstrated that low energy electron microscopy (LEEM) is well suited to image surfaces of crystallites and grain boundaries intersecting the surface of polycrystals. In this contribution we report on our application of LEEM to monitor segregation and diffusion processes at the surface of polycrystalline Fe samples. During thermal treatment of the Fe polycrystal, we observed formation of islands which consisted of bulk impurities segregated to the surfaces of the crystallites. Depending on temperature ramp and surface orientation of the crystallites, different shapes of these islands were observed. At elevated temperatures Ostwald ripening of the impurity islands occurred. Increasing the temperature even more caused dissolution of these islands via diffusion into the bulk of the polycrystal, mainly along grain boundaries. In the majority of these transformations the polycrystalline texture remained unaffected by segregation and diffusion processes, but we also observed grain boundary motion.

O 7.3 Mon 11:45 WIL C107

Ultrafast melting of a charge-density wave in the Mott insulator 1*T*-TaS_2 — •Stefan Hellmann, Christian Sohrt, Timm Rohwer, Matthias Kalläne, Michael Bauer, Lutz Kipp, and Kai Rossnagel — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany

Femtosecond time-resolved core-level photoemission spectroscopy with the free-electron laser FLASH as well as time- and angle-resolved photoemission spectroscopy with a higher-harmonics-generation source are used to measure the atomic-site and momentum specific charge-order dynamics of the charge-density wave in the Mott insulator 1*T*-TaS_2. After strong photoexcitation, melting of the charge-density wave and the accompanying periodic lattice disortion is observed on two timescales. The subsequent fast electron-phonon thermalization drives the system across a phase transition from a long-range charge ordered state to a quasi-equilibrium state with domain-like short-range charge and lattice order. The combination of the two complementary sources opens the way to study the nonequilibrium dynamics of condensed matter systems with full momentum, elemental, chemical, and atomic-site selectivity.

O 7.4 Mon 12:00 WIL C107

Waveguiding of hot surface state electrons by the Au(111) reconstruction — •Viktor Geringer[1,2], Dinesh Subramaniam[1,2], Florian Libisch[3], Marcus Liebmann[1,2], and Markus Morgenstern[1,2] — [1]II. Institute of Physics, RWTH Aachen University, Otto-Blumenthal-Str., 52074 Aachen, Germany — [2]JARA: Fundamentals of Future Information Technology — [3]Institute for Theoretical Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10/136, A-1040 Vienna, Austria

Using scanning tunneling spectroscopy (STS) we perform a spatial and energy dependent study of the electronic scattering behavior on the Au(111) surface. In spite of the small surface reconstruction potential (35 meV), our measurements reveal a surprising effect of wave guiding. Electrons with energies up to twenty times larger than the corrugation of the potential follow the geometry of the reconstruction, observable through a strong anisotropy in the distribution of the wave vectors. In order to explain this behavior we calculated the square of the electronic wave function evidencing quantum-mechanical orthogonality as the origin of the waveguiding effect.

O 7.5 Mon 12:15 WIL C107

Kinetic energy distributions of vibrationally promoted electrons at metal surfaces: Comparison of different initial vibrational states — •Tim Schäfer[1], Jerry Larue[2], Daniel Matsiev[2], Luis Velarde[2], Daniel J. Auerbach[2], and Alec M. Wodtke[1] — [1]Georg-August Universität Göttingen, Institut für Physikalische Chemie, Tammannstr.6, 37077 Göttingen, Germany — [2]Department of Chemistry and Biochemistry, University of California, Santa Barbara, CA 93106-9510, USA

Kinetic energy distributions of exoelectrons produced by collisions of highly vibrationally excited NO molecules with a low work function Cs dosed Au surface were studied. The NO molecules were optically prepared in $X^2\Pi_{1/2}$ (v=16) and $X^2\Pi_{1/2}$ (v=22) using Stimulated Emission Pumping (SEP) and the electron energy distributions were measured with a home-built retarding field electron energy analyzer. The results obtained by these experiments indicate that many quanta, as high as Δv =17 for v=22, can be transferred to a single electron. The most probable transfer of vibrational quanta is Δv =11 for NO(v=16) and Δv = 12 for NO(v=22) and is in qualitatively good agreement with previous studies. In addition to the results obtained by the experiments with the SEP prepared molecules the study of vibrationally excited molecules produced by spontaneous emission (Franck-Condon pumping, FCP) supports the overall conclusion: The kinetic energy distribution of vibrationally promoted electrons strongly suggests a coupling of multiple vibrational quanta to a single electron and cannot be explained in a simple adiabatic picture.

O 7.6 Mon 12:30 WIL C107

Optimal control of open quantum systems applied on photochemistry on surfaces — Erik Asplund and •Thorsten Klüner — Carl von Ossietzky Universität Oldenburg, Germany

A quantum system in condensed phase, which undergoes strong dissipative processes, is an open quantum system. From the theoretical viewpoint it is important to model open quantum systems in a rigorous way. The description of open quantum systems can be realized within the "Surrogate Hamiltonian" approach, which is a non-Markovian approach. In the "Surrogate Hamiltonian" approach, a quantum system is separated into a primary system and a bath. Besides the traditional formulation of dissipative processes through the spectral density, the "Surrogate Hamiltonian" method enables a microscopic description of excitation and relaxation process for open quantum systems.

Light interacting with atoms and molecules is not only a source of information about the atoms and molecules studied, it can also initiate charge and energytransfer processes, i.e. manipulate the evolution of the molecules studied. A theoretical tool for the design of laser pulses to transfer an initial state to a final state is optimal control theory (OCT). Besides the traditionalfinal-time control algorithms, there exist methods to also handle time-dependent control targets. In this talk, OCT with time-dependent targets is combined with the "Surrogate Hamiltonian" method in order to gain control of dissipative quatum systems. Two model systems representing adsorbate-surface systems will be presented and the controllability of the systems will be discussed.

O 7.7 Mon 12:45 WIL C107

Rotational and constitutional dynamics of caged supramolecules — •Florian Klappenberger[1], Dirk Kühne[1], Wolfgang Krenner[1], Svetlana Klyatskaya[2], Mario Ruben[2], and Johannes V. Barth[1] — [1]Physik Department E20, TU München, Germany — [2]Institute of Nanotechnology, Forschungszentrum Karlsruhe, Karlsruhe, Germany

The confinement of guest species in nanoscale environments leads to dynamic phenomena. Notably the organization and rotational motions of individual molecules were controlled by carefully designed, fully supramolecular host architectures. Here we use an open 2D coordination network on a smooth metal surface to steer the self-assembly of discrete trimeric guest units, identified as noncovalently bound dynamers. Each caged chiral supramolecule performs concerted, chirality-preserving rotary motions within the template honeycomb pore, which are visualized and quantitatively analyzed using temperature-controlled scanning tunneling microscopy. Furthermore, with higher thermal energies, a constitutional system dynamics appears, which is revealed by monitoring repetitive switching events of the confined supramolecules chirality signature, reflecting decay and reassembly of caged units.