

O 12: Symposium: Size-Selected Clusters at Surfaces I (Invited Speakers: Karl-Heinz Meiwes-Broer, Heinz Hövel, Thorsten Bernhardt)

Time: Monday 13:30–16:45

Location: MA 005

Invited Talk

O 12.1 Mon 13:30 MA 005

Charge transport and magnetism of deposited clusters — ●KARL-HEINZ MEIWES-BROER¹, INGO BARKE¹, ARMIN KLEIBERT¹, VIOLA VON OYENHAUSEN¹, JOACHIM BANSMANN², KRISTIAN SELL¹, STEFAN POLEI¹, and NORMAN WILKEN¹ — ¹Institut für Physik, Universität Rostock, Universitätsplatz 3, D-18051 Rostock, Germany — ²Abteilung Oberflächenchemie und Katalyse, Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm, Germany

Magnetism and electronic properties of clusters at surfaces are of wide interest as is documented by the current Priority Programme of the Deutsche Forschungsgemeinschaft (DFG-Schwerpunktprogramm 1153) [1]. In particular, the novel physics found on the nm-scale might lead to interesting novel objects for future applications. In this contribution 3 to 15 nm mass-filtered metal clusters are studied deposited from an ACIS source onto ultraclean solid surfaces. In the case of alloy clusters, the particles stoichiometry could independently be clarified by EDX and X-ray absorption spectroscopy, typically yielding a composition close to the target material. Low-temperature STS serves for the investigation of electronic properties. The resulting dI/dU curves are distinctly structured which results from the size-dependent density of states of the clusters as well as from the underlying substrate. Magnetic properties are interrogated with x-ray absorption (XMCD) measurements. Strongly size and substrate dependent magnetic orbital moments are found [2].

- [1] Special issue on clusters at surfaces in Appl. Phys. A 82(1), 2006
[2] A. Kleibert et al., J. Appl. Phys. 101, 114318, 2007

Invited Talk

O 12.2 Mon 14:00 MA 005

Supported Magic Numbers for Size-Selected Ag Clusters on Fullerene Layers — ●H. HÖVEL¹, S. DUFFE¹, L. PATRYARCHA¹, T. RICHTER¹, B. SIEBEN¹, C. YIN², B. VON ISSENDORFF², and M. MOSELER^{3,4} — ¹Technische Universität Dortmund, Experimentelle Physik I — ²Universität Freiburg, Fakultät für Physik — ³Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg — ⁴Freiburg Materials Research Center

Mass selected clusters from Ag₅₅⁺ to Ag_{561±5}⁺ were deposited on HOPG and Au(111) functionalized with monolayers (ML) of C₆₀ molecules, which proved to be a new and promising choice for the investigation of mass selected clusters. Depositions at 165 K gave extremely narrow cluster height distributions in STM images measured at 77 K. Molecular dynamics simulations for the deposition suggest softlanding with minor distortions of the icosahedral cluster shape at the cluster-fullerene interface [1]. Using C₆₀/HOPG or 2 ML C₆₀/Au(111) the cluster heights are stable for more than 12 h at room temperature (RT). For 1 ML C₆₀/Au(111) the cluster height decreases and finally all clusters disappear at RT. Molecular dynamics simulations reveal a process by which the clusters decay atom by atom through 1 ML C₆₀/Au(111) at RT. A sharp maximum at 1.7 nm cluster height forms during the cluster decay, indicating that there exists some metastable 'supported magic number'. For the soft-landed clusters we measured identical spectral features for individual clusters with the same selected size using STS at 5 K.

- [1] S. Duffe et al., Eur. Phys. J. D (2007), published online

Invited Talk

O 12.3 Mon 14:30 MA 005

Femtosecond laser spectroscopy of clusters at surfaces — ●THORSTEN M. BERNHARDT — Institut für Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm, Germany

Femtosecond two photon photoemission spectroscopy is employed to investigate the electronic structure of ultra-thin magnesium oxide films and of mass-selected clusters deposited onto this substrate. Distinct changes in the electronic structure of these films induced by oxygen vacancy defects and by metal cluster deposition are identified in the photoemission spectra and help to elucidate the origin of the observed catalytic activity of supported cluster nano-systems. Furthermore, in a new experimental approach, time-of-flight mass spectrometry in conjunction with femtosecond resonance-enhanced multiphoton ionization is used to directly monitor the chemical reaction dynamics of adsorbate molecules. This new method enables the distinction of different reaction pathways through direct real-time monitoring of the mass and

the kinetic energy of reaction products and intermediates.

15 min. break

O 12.4 Mon 15:15 MA 005

Mass-selected non-IPR fullerenes deposited on HOPG — ●DANIEL LÖFFLER, PATRICK WEIS, ARTUR BÖTTCHER, and MANFRED M. KAPPES — Institut für Physikalische Chemie, Universität Karlsruhe (TH), Germany

C_n layers, (48 ≤ n ≤ 68), have been created under ultra high vacuum conditions by low-energy deposition of mass-selected C_n⁺ clusters onto HOPG surfaces [1][2]. C_n⁺ (48 ≤ n ≤ 68) ions originate from the electron-impact induced ionization and fragmentation of C₆₀ and C₇₀. The resulting C_n cages represent non-IPR building blocks (Isolated Pentagon Rule) and exhibit localized reaction centers (e.g. adjacent pentagons, 2AP, heptagonal rings, HP, squares). This property leads to the formation of covalent intercage bonds, -C_n-C_n-, which are responsible for the high thermal stability of the C_n solid films. The activation energy for desorption of C_n is considerably higher than the value found for related IPR cages. The intercage binding energies found for C_n⁺ (62 ≤ n ≤ 68) are lower than those found for the corresponding C_n⁺ (50 ≤ n ≤ 58) cages. This fact indicates that the strength of the C_n-C_n bonds results from the interplay between the cage curvature (pyramidal angle) and the mean number of non-IPR reaction centers per cage. The electronic structure of the valence band, as monitored by UPS (21.2eV), varies significantly with the cage size. The surface ionization potential and the width of the HOMO-LUMO gap dependent on the cage size and on the type of non-IPR sites terminating the cage.

- [1] Böttcher et al., PCCP, 7 (2005) 2816
[2] D. Löffler et al., J. Chem. Phys. 125 (2006) 224705

O 12.5 Mon 15:30 MA 005

Counting electrons in quantum-well states of Au chains on an alumina thin film on NiAl — ●MARIA VERONICA GANDUGLIA-PIROVANO¹, NIKLAS NILIUS², VERONIKA BRAZDOVA¹, MARIA KULAWIK², JOACHIM SAUER¹, and HANS-JOACHIM FREUND² — ¹Institut für Chemie, Humboldt-Universität zu Berlin, Berlin, Germany — ²Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Low-temperature STM measurements combined with DFT calculations are employed to study the adsorption of gold on alumina/NiAl(110). The binding of Au monomers involves breaking of an oxide Al-O bond below the adatom and stabilizing the hence under-coordinated O ion by forming a new bond to an Al atom in the NiAl. The adsorption implies negative charging of the adatom. The linear arrangement of favorable binding sites induces the self-organization of Au atoms into chains. Their electronic structure is described by a series of quantum well states (QWSs) that evolve from the *s-d_{z2}* orbitals of the single adatoms. The node structure of the QWSs can only be explained when considering the charge transfer through the thin alumina film into the Au adchains in the electron count.

- [1] N. Niliius, M. V. Ganduglia-Pirovano, V. Brázdoová, M. Kulawik, J. Sauer, and H-J. Freund, Phys. Rev. Lett. submitted.

O 12.6 Mon 15:45 MA 005

Unoccupied states of individual silver clusters and chains on Ag(111) — ●ALEXANDER SPERL¹, JÖRG KRÖGER¹, NICOLAS NEÉL¹, HENNING JENSEN¹, RICHARD BERNDT¹, ANDREAS FRANKE², and ECKHARD PEHLKE² — ¹Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — ²Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Size-selected silver clusters on Ag(111) were fabricated by single-atom manipulation using the tip of a low-temperature scanning tunneling microscope. Unoccupied electron resonances give rise to spectral features which shift towards the Fermi level with increasing cluster size. Linear assemblies exhibit higher resonance energies than equally sized compact assemblies. Density functional theory calculations reproduce the observed energies for the linear clusters and enable an assignment

of the resonances to hybridized atomic 5s and 5p orbitals with silver substrate states.

O 12.7 Mon 16:00 MA 005

Size-dependent Surface States on Strained Cobalt Nanoislands on Cu(111) — ●BENJAMIN HEINRICH¹, MIRCEA-VASILE RASTEI¹, LAURENT LIMOT¹, PAVEL A. IGNATIEV², VALERI S. STEPANYUK², PATRICK BRUNO², and JEAN-PIERRE BUCHER¹ — ¹Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, Université Louis Pasteur, F-67034 Strasbourg, France — ²Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle/Saale, Germany

Nanoislands on metal surfaces have been a matter of intense research for decades in view of prospective applications in a vast variety of domains. One of the main challenges in this regard is to control the interplay between the physical properties, whether magnetic, electronic or chemical, and the lattice mismatch with the metal substrate, which results in changes due to strain.

In this work, we focus on the interplay between strain relaxations and the surface states of Co nanoislands on Cu(111). By low-temperature scanning tunneling spectroscopy (LT STS), taken over the islands, we show for the first time that the electronic states of the islands vary with their size: Occupied surface states exhibit a sizeable downward energy shift as the island size decreases. Atomic-scale simulations and *ab initio* calculations confirm that the driving force for the observed shift is related to size-dependent mesoscopic relaxations in the nanoislands.

O 12.8 Mon 16:15 MA 005

Thermally activated processes for mass selected Ag clusters on 1 and 2 monolayers C₆₀ on Au(111) — ●S. DUFFE¹, L. PATRYARCHA¹, T. RICHTER¹, B. SIEBEN¹, H. HÖVEL¹, C. YIN², B. VON ISSENDORFF², and M. MOSELER^{3,4} — ¹Technische Universität Dortmund, Experimentelle Physik I — ²Universität Freiburg, Fakultät für Physik — ³Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg — ⁴Freiburg Materials Research Center

We deposited at 165 K mass selected clusters from Ag_{147±1} to Ag_{561±5}, expected to form geometrically magic icosahedra, on 1.7 ML

C₆₀/Au(111). On 1 and 2 ML C₆₀ we observed very narrow cluster height distributions. After annealing, the clusters on 2 ML C₆₀ kept their original height for more than 12 hours at room temperature (RT). In contrast the clusters on 1 ML C₆₀ decayed and disappeared at RT [1]. During the decay process we observed a metastable size with the height of 1.7 nm for different initial cluster sizes. Neither Ag₅₅ with h=(1.5 ± 0.2) nm nor Ag₁₄₇ with h=(2.0 ± 0.2) nm after deposition at 165 K corresponded to the peak at h=1.7 nm. Therefore we deposited Ag₈₀ and Ag₆₈ at 165 K and observed cluster heights of ≈ 1.5 nm on 1 and 2 ML C₆₀ for both cluster sizes, probably due to their prolate shape. The subsequent annealing of the clusters up to RT caused a change of the cluster height distribution, probably due to Ostwald ripening, and the metastable size with the height of 1.7 nm was formed. Thus mass selected geometrically non-magic Ag clusters show a different behavior at RT as geometrically magic Ag clusters.

[1] S. Duffe et al., Eur. Phys. J. D (2007), published online

O 12.9 Mon 16:30 MA 005

Structure and properties of deposited size selected Fe₅₀Co₅₀ alloy clusters — ●WOLFGANG ROSELLEN, FURKAN BULUT, RENATE KERSTIN GEBHARDT, and MATHIAS GETZLAFF — Institut für Angewandte Physik, Universitätsstr.1 D-40225 Düsseldorf

Size-selected Fe₅₀Co₅₀ alloy cluster were generated by a continuously working Arc Cluster Ion Source (ACIS). The selection is carried out by means of an electrostatic quadrupole. The typical size of the clusters is between 6-12nm. The lateral size distribution and the crystalline properties were investigate ex-situ by means of High Resolution Transmissions Electron Microscopy (HRTEM). The alloy clusters were deposited on a tungsten W(110) surface under UHV condition in order to avoid oxidation. The distribution of height and size were determined by scanning tunnelling microscopy (STM) experiments for different sizes of the incoming particles and several deposition angles with respect to the W(110) surface. Additionally, the structural properties of *individual* Fe₅₀Co₅₀ clusters were examined.

• [1] M. Getzlaff et al., Appl. Phys. A 82 (2006) 95

• [2] K. Gebhardt et al., Eur. Phys. J. D (submitted)