O 50: Poster: Nanostructures on Surfaces II

Time: Tuesday 18:15–20:30 Location: Poster B

O 50.1 Tue 18:15 Poster B

Vibrational properties of the Au-($\sqrt{3}\times\sqrt{3}$)/Si(111) surface reconstruction — •S. Sanna[1], M. Krenz[2], S. Neufeld[2], W. G. Schmidt[2], E. Speiser[3], J. Räthel[3], S. Chandola[3], N. Esser[3], B. Halbig[4], M. Liebhaber[4], U. Bass[4], and J. Geurts[4] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen — [2]Department Physik, Universität Paderborn — [3]Leibniz-Institut für Analytische Wissenschaften, Berlin — [4]Physikalisches Institut, Experimental Physics 3, Universität Würzburg

The atomic structure of the Au-induced $\sqrt{3}\times\sqrt{3}$ reconstruction of the Si(111) surface has been controversially discussed for two decades. Different structural models have been proposed to explain the observed STM Pattern [J. Phys. Condens. Matter **27**, 475001 (2015)]. While the proposed structural models are almost energetically degenerate, the analysis of the vibrational properties might help to assign a structural model to the surface reconstruction. Our first principles calculations within density functional theory predict surface localized phonon modes for all investigated structures. However, the calculated Raman spectra are model-dependent. Corresponding surface Raman measurements reveal the presence of vibrational eigenmodes in the spectral range from 20 to 450 cm^{-1}, which are compatible with the frequencies calculated for the conjugate honeycomb-chained-trimer model (CHCT) [Surf. Sci. 275, **L691** (1992)]. On the basis of the phonon eigenfrequencies, symmetries, and Raman intensities, we assign the measured spectral features to the calculated phonon modes.

O 50.2 Tue 18:15 Poster B

Density functional theory investigation of rare earth silicide nanowires — •Kris Holtgrewe[1], Wolf Gero Schmidt[2], and Simone Sanna[1] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, D-35392 Gießen — [2]Department Physik, Universität Paderborn, Warburger Str. 100, D-33098 Paderborn

Quasi one-dimensional electron systems are of fundamental interest both because of their unusual physical properties and for devices on nanometer scale. A prototype for these systems are rare earth (RE) silicide nanowires on silicon(001) surfaces. They grow self-organized controlled by macroscopic parameters such as temperature and amount of deposited RE.

Unfortunately, the knowledge about nanowires' detailed atomic structure, which is crucial for understanding their physical properties, is still incomplete. We have investigated different wire models from first-principles within density functional theory (DFT). Thereby erbium is chosen as a prototypical trivalent rare earth ion, its 4f-electrons treated as frozen states in the atomic core.

We categorized the models corresponding to six degrees of freedom: width, height, depth of burial, unit cell orientation, roof reconstruction and the underlying bulk RE silicide structure (hexagonal/tetragonal). After comparing the formation energy within ab-initio thermodynamics, electronic band structures and densities of states are calculated for the stable wires. Structural and electronic properties are discussed and compared with available STM, STS and ARPES measurements.

O 50.3 Tue 18:15 Poster B

Atomic-scale Au chains on Si(553): Influence of Defects — •Christian Braun and Wolf Gero Schmidt — Universität Paderborn, Paderborn, Germany

One-dimensional atomic-scale metallic nanowires are popular model systems to study phenomena of one-dimensional physics such as Peierls instabilities, spin-charge separation, and charge-density waves [1]. Defects may be used to tune the nanowire properties, e.g., the electron transport or phase transition temperature. Recently it was shown that additional Si adatoms on Si(775)-Au induce local spin-polarization at the step [2]. In the present work the influence of Si adatoms and small molecules on the atomic structure and electronic properties of Si(553)-Au is investigated. For that purpose, density functional theory calculations are combined with ab initio thermodynamics. We discuss the defect impact on the Au chain dimerization, electronic band structure and predict desorption temperatures for foreign adsorbates.

[1] T Frigge, B Hafke, T Witte, B Krenzer, C Streubühr, A Samad Syed, V Miksic Trontl, I Avigo, P Zhou, M Ligges, D von der Linde, U Bovensiepen, M Horn-von Hoegen, S Wippermann, A Lücke, S Sanna, U Gerstmann, WG Schmidt, Nature 544, 207 (2017)
[2] J Aulbach, SC Erwin, R Claessen, J Schäfer, Nano Letters 16, 2698-2704 (2016)

O 50.4 Tue 18:15 Poster B

Spectral signatures of spin-charge separation in MoS_2 mirror twin boundaries — •Philipp Weiss[1], Wouter Jolie[2,3], Clifford Murray[2], Joshua Hall[2], Arkady Krasheninnikov[4], Hannu-Pekka Komsa[5], Carsten Busse[2,3,6], Thomas Michely[2], and Achim Rosch[1] — [1]Institute for Theoretical Physics, University of Cologne, Germany — [2]Institute of Physics II, University of Cologne, Germany — [3]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [5]Department of Applied Physics, Aalto University, Finland — [6]Department Physik, Universität Siegen, Germany

We calculate the local spectral density of a one-dimensional metallic wire of finite length as predicted by Luttinger liquid theory. Fourier transformation in space yields the linear dispersion of spin and charge density waves which are the fundamental excitations of the system.

We apply this theory to recent STM measurements in MoS_2 mirror twin boundaries. Due to the metallic nature of these one-dimensional structures one can expect to find signatures of spin-charge separation in the STM signal. By means of the Fourier analysis we are able to extract spin and charge velocities from the experimental data. This indicates that a Luttinger liquid is likely realized in such grain boundaries.

O 50.5 Tue 18:15 Poster B

Gold-induced Surfaces on Stepped Germanium: Towards Atomic Models — •Tim Wagner, Julian Aulbach, Ralph Claessen, and Jörg Schäfer — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg

Self-assembly of gold atoms on terraced Si(hhk) or Ge(hhk) substrates stabilizes certain surface orientations. While Si(553)-Au and Si(557)-Au have already been thoroughly examined, showing honeycomb step edges with regular arrays of spins, the atomic structure of the related Ge(hhk)-Au systems has not yet been determined. In order to investigate the influence of the substrate on the atomic structure, we perform scanning tunneling microscopy and low energy electron diffraction measurements on Ge(hhk)-Au surfaces. Based on our results, we propose first atomic structure models for Ge(221)-Au, Ge(335)-Au and Ge(557)-Au taking into account the known structural motifs of the Si(hhk)-Au family [1] and of the metal-induced Ge(111)-M systems [2]. While the Ge(335)-Au and Ge(557)-Au surface reconstructions display a great resemblance to their Si(hhk)-Au counterparts, in the special case of Ge(221)-Au the missing registry shift between neighboring step edges imposes an unusual rectangular unit cell, giving rise to a potentially different kind of inter-step correlation.

[1] J. Aulbach et al., Nano Lett. 16(2698) (2016).
[2] A. Tomaszewska et al., Ultramicroscopy 111(392) (2011).

O 50.6 Tue 18:15 Poster B

Temperature-dependent order-disorder transition in the Si(553)-Au nanowire system — •Bernd Hafke, Tim Frigge, Tobias Witte, Boris Krenzer, and Michael Horn-von Hoegen — Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg

Deposition of 0.5 ML Au on Si(553) at 650 °C results in the formation of Au double-strand chains with a twofold periodicity along the terraces of the vicinal Si surface. These metallic wires are structurally terminated by Si step edge atoms, where every third atom exibits a dangling bond leading to a threefold periodicity. Theory predicts magnetic properties of these interacting half-filled Si step edge atoms [1,2]. The long-range interaction of the twofold and threefold periodicity is investigated by spot-profile analysis in LEED at sample temperatures between 60 K and 180 K. The correlation length of Si step edge atoms along and perpendicular to the steps abruptly decreases upon heating above a temperature of $T \approx 100$ K, respectively. Interestingly, the streak-like intensity, indicative for the twofold periodicity of the Au atoms, shows an opposite behavior, i.e., an increase in correlation lenth upon heating. These findings are explained within a scenario of an order-disorder transition accompanied with the creation of so-called heavy and light zerodimensional domain boundaries.

[1] S. C. Erwin and F. J. Himpsel, Nature Commun. **1**, 58 (2010).
[2] B. Hafke, *et al.* PRB **94**, 161403(R) (2016).

O 50.7 Tue 18:15 Poster B

Coupling of structural and electronic properties in 4/3-ML Pb/Si(111) investigated by femtosecond time- and angle-resolved 2PPE

— •Abdul Samad Syed, Manuel Ligges, Vesna Mikšić Trontl, Peter Kratzer, and Uwe Bovensiepen — Fakultät für Physik, Universität Duisburg-Essen, Germany

Electronic properties and atomic structure of low dimensional systems determine each other. Scattering at steps was found, e.g., for Pb/Si(557) to lead to different electron relaxation for step down and step up directions [1]. A related, problem appears for threefold symmetry of Pb/Si(111)-($\sqrt{3}\times\sqrt{3}$) and we report here on the unoccupied electronic structure along $[\overline{1}\overline{1}2]$ and $[11\overline{2}]$ investigated by femtosecond time- and angle-resolved two photon photoemission (2PPE). Three electronic features dispersing along $k_x \parallel [\overline{1}\overline{1}2]$ were identified with binding energies 3.65, 3.5, and 3.3 eV above the Fermi level. In angle-resolved measurements the observed electronic states show for opposite momenta $k_x > 0$ and $k_x < 0$, an asymmetric intensity $I(k_x)$ and the electronic structure that appears to be different. In time-resolved experiment we find a momentum dependent change in the electron relaxation time $\tau(k_x)$. Polarization dependent studies reveal a different orbital character for the different states and for opposite k_x. We conclude to have identified the unidirectional anisotropy in the real and imaginary part of the electron self energy originating from the threefold surface symmetry of Pb/Si(111)-($\sqrt{3}\times\sqrt{3}$).

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[1] A. Samad Syed et al., Phys. Rev. B **92**, 134301 (2015).