

## O 95: Semiconductor Substrates: Metallic Nanowires

Time: Friday 10:30–13:00

Location: H14

O 95.1 Fri 10:30 H14

**Novel electronic junctions in an atomic wire array: interfaces between metallic and charge density wave ordered electronic phases** — ●SAMAD RAZZAQ<sup>1</sup>, SUN KYU SONG<sup>2</sup>, HAN WOONG YEOM<sup>3</sup>, and STEFAN WIPPERMANN<sup>4</sup> — <sup>1</sup>Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — <sup>2</sup>Center for Artificial Low D Electronic Systems, Pohang, S.Korea — <sup>3</sup>Center for Artificial Low D Electronic Systems, Pohang, S.Korea — <sup>4</sup>Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The Si(111)-(4x1)In atomic wire array is an extremely popular model for one-dimensional electronic systems. It features a reversible, temperature-induced metal insulator transition into a charge density wave (CDW) ordered ground state with (8x2) translational symmetry. Close to the phase transition temperature, both phases can co-exist and form novel types of electronic junctions between the metallic (4x1) phase and the insulating CDW-ordered (8x2) phase. Combining scanning tunneling microscopy/spectroscopy (STM/STS) and ab initio molecular dynamics calculations, we explore the microscopic structure of interfaces between distinct electronic phases at the atomic scale. Specific defects allow to modify and control the structure of these electronic interfaces. We explain the atomistic mechanism behind the junction formation and its tunability from first principles. Financial support from the German Research Foundation (DFG), grant no. FOR1700 is gratefully acknowledged.

O 95.2 Fri 10:45 H14

**Coherent control of the structural phase transition in In-nanowires on Si(111)** — ●JAN GERIT HORSTMANN, BARELD WIT, GERO STORECK, and CLAUDIUS RUPERS — IV. Physical Institute, University of Göttingen, Friedrich-Hund-Platz 1, Germany

Metallic nanowires have become a model system for studying correlation effects and light-matter interaction on the atomic scale, providing access to phenomena such as anisotropic conductivity, long-range spin-order or Peierls transitions. Due to their low dimensionality, these systems exhibit a comparatively small number of structural modes, potentially resulting in long dephasing times of optically-excited coherent phonons. Recently, it was shown that single intense light pulses can drive the surface-specific structural phase transition between the insulating (8x2) and the metallic (4x1) phase of In-nanowires on Si(111) in the limit of critically damped atomic motion [1]. Here, we report the coherent control of this structural phase transition enabled by excitation with optical pulse pairs, thereby demonstrating and harnessing pronounced vibrational coherences in the system. A detailed analysis of the phase transition efficiency as a function of the two-pulse delay recorded by ultrafast low-energy electron diffraction (ULEED) [2] proves the critical role of two specific phonon modes for the transition [3], and allows for unique insights to the underlying reaction pathways of this structural phase transition.

[1] T. Frigge et al., *Nature* 544, 207-211 (2017). [2] S. Vogelgesang et al., *Nat. Physics* 14, 184-190 (2018). [3] S. Wippermann et al., *PRL* 105, 126102 (2010).

O 95.3 Fri 11:00 H14

**Excited state mapping and ultrafast population dynamics in In/Si(111) nanowires probed by trARPES** — ●CHRIS W. NICHOLSON<sup>1</sup>, MICHELE PUPPIN<sup>1</sup>, ANDREAS LÜCKE<sup>2</sup>, WOLF GERO SCHMITT<sup>2</sup>, LAURENZ RETTIG<sup>1</sup>, RALPH ERNSTORFER<sup>1</sup>, and MARTIN WOLF<sup>1</sup> — <sup>1</sup>Fritz Haber Institute, Berlin — <sup>2</sup>University of Paderborn

Ultrafast electronic structure probes allow detailed insights into the microscopic processes underlying photo-induced phase transitions, as recently exemplified by the time- and angle-resolved photoemission spectroscopy (trARPES) study of the model (8x2) to (4x1) structural transition in In/Si(111) nanowires [1].

In this talk, I will address two further aspects of the electronic structure dynamics as probed by our trARPES setup utilizing a 22 eV laser at 500 kHz. The first is the extension of the band-mapping concept to states above the Fermi level, which allows a rigorous benchmarking of band structure calculations in this system. The second is an energy and momentum resolved analysis of the population dynamics during the phase transition. A comparison with a simulated band structure based on a transient electronic temperature finds impressive agreement, supporting the high electronic temperature extracted in

the surface layer following excitation. These results are compared to those obtained with femtosecond electron diffraction [2] and imply a non-thermal phonon population of the surface In atoms and suggest a bottleneck for cooling of optical phonons.

[1] Nicholson et al. *Science* 362, 821 (2018)  
[2] Frigge et al. *Struct. Dyn.* 5, 025101 (2018)

O 95.4 Fri 11:15 H14

**1D- plasmons and their H-induced modification on the Si(557)-Au surface** — ●ZAMIN MAMIYEV<sup>1</sup>, SIMONE SANNA<sup>2</sup>, CHRISTOPH TEGENKAMP<sup>1</sup>, and HERBERT PFNÜR<sup>1</sup> — <sup>1</sup>Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany — <sup>2</sup>Theoretische Physik, Justus-Liebig-Universität Gießen, Gießen

Recently significant progress has been made on metallic atomic wires on the stepped Si surfaces. However, there are still fundamental questions concerning substrate wire interaction, tunability in atomic scale et.c. need to be clarified. Such wires host anisotropic plasmonic excitations which contain significant information about excited states and also have a potential application in nano-optoelectronics. Here we use plasmon spectroscopy and atomistic DFT calculations to study the H-induced modifications of quasi-1D plasmons in Au atomic wires on the Si(557) surface. Single atomic Au chains per terrace form upon evaporation of 0.19ML Au onto this surface while emerging other structural motifs with an individual chemical potential. Adsorption of atomic H induces a reduction of dispersion and levelling of the dispersion around 0.45 eV for  $k_{\parallel} > 0.08 \text{ \AA}^{-1}$ , indicative of band gap opening in the unoccupied part of the band structure. No extrapolation to  $E=0$  at  $k_{\parallel} = 0$  is possible any more, indicating increased electronic localization and/or influences by disorder. These findings are corroborated by DFT calculations, which predict adsorption of H first on the Si step edge and then on the Si rest atom row. Using the relation between e-h continuum and plasmon dispersion, the modification of band structure and its consequences on plasmonic excitation will be discussed.

O 95.5 Fri 11:30 H14

**Temperature induced phase transition of Si(553)-(5x2)-Au in vibrational spectra and its suppression upon step edge hydrogenation** — ●EUGEN SPEISER<sup>1</sup>, JULIAN PLAICKNER<sup>1</sup>, SANDHYA CHANDOLA<sup>1</sup>, SIMONE SANNA<sup>2</sup>, CONOR HOGAN<sup>3</sup>, and NORBERT ESSER<sup>1</sup> — <sup>1</sup>Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V. Schwarzschildstrasse 8, 12489 Berlin, Germany — <sup>2</sup>Institut für Theoretische Physik, Heinrich-Buff-Ring 16, 35392 Gießen — <sup>3</sup>Istituto di Struttura della Materia-CNR (ISM-CNR), via Fosso del Cavaliere 100, 00133 Rome, Italy

Si(553)-(5x2)-Au is known for its combined structural/electronic phase transition, confirmed by calculations and experiments. Its investigation by vibrational spectroscopies is promising due to their unique sensitivity to atomic scale properties. By comparison to DFT calculations, certain modes in vibrational spectra are assigned to the Si step edge and hence can be used for probing its properties. Indeed, we observe a temperature induced change in vibrational modes at the step edge. The properties of this system are governed by the charge distribution between step edge and Au-chain. As shown previously hydrogenation of the step edge opens the possibility to use it for manipulation of charge distribution. We show that hydrogenation of the step edge suppresses the phase transition related change in vibrational modes. A tentative explanation will be given in terms of thermally induced fluctuation in the charge distribution for the non-hydrogenated surface. This fluctuation is inhibited by additional charge, introduced by hydrogen, suppressing the phase transition.

O 95.6 Fri 11:45 H14

**Temperature-dependent order-disorder transition in the Si(553)-Au nanowire system** — ●BERND HAFKE<sup>1</sup>, TOBIAS WITTE<sup>1</sup>, CHRISTIAN BRAND<sup>1</sup>, SIMONE SANNA<sup>2</sup>, CHRISTIAN BRAUN<sup>3</sup>, WOLF GERO SCHMIDT<sup>3</sup>, and MICHAEL HORN-VON HOEGEN<sup>1</sup> — <sup>1</sup>Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg — <sup>2</sup>Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — <sup>3</sup>Universität Paderborn, Pohlweg 55, 33098 Paderborn

Deposition of 0.5 ML Au on Si(553) at 650 °C results in the formation of Au double-strand metallic chains with a twofold periodicity along the terraces of the vicinal Si surface. The step edge atoms of the Si

terraces are characterized by a threefold periodicity, due to the presence of unoccupied dangling bonds [1,2]. The long-range interaction of the twofold and threefold periodicity is investigated by spot-profile analysis in LEED as function of temperature between 60 K and 190 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. These findings are explained within a scenario of an order-disorder transition, where the thermal creation of solitons destroy the long-range ordering. Additionally, time-resolved ultra-fast RHEED experiments show the streak-like intensity, indicative for the twofold periodicity of the Au atoms, to decrease upon intense fs-optical excitation. This indicates transient weakening of the dimerization within the Au double-strand.

[1] S. C. Erwin and F. J. Himpsel, *Nature Commun.* **1**, 58 (2010).

[2] C. Braun, *et al.* *PRB* **98**, 121402 (2018).

O 95.7 Fri 12:00 H14

**Spin pairing versus spin chains at Si(*hkk*)-Au surfaces** — ●CHRISTIAN BRAUN and WOLF GERO SCHMIDT — Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn

Surfaces involving single spin states are promising candidates for the realization of spin-based computation and storage. Both the Si(553)-Au and Si(557)-Au surface have been discussed to exhibit such unpaired spins for several years [1]. Density-functional theory is used to probe the spin structure of these surfaces. For Si(553)-Au a diamagnetic  $sp^2 + p$  rehybridized structure, where the dangling bonds are either filled with two spin-paired electrons or are empty, is more favorable and in better agreement with experiment than the generally accepted spin-chain model. In contrast, the spin chains on Si(557)-Au seem rather stable against rehybridization. We discuss the mechanisms for this diverging behavior and predict methods to tailor the existence of single spin states on these surfaces. [2]

[1] S C Erwin, F J Himpsel, *Nature Communications* **5**, 58 (2010)

[2] C Braun, U Gerstmann, W G Schmidt, *Physical Review B* **98**, 121402 (2018)

O 95.8 Fri 12:15 H14

**Phenomenological assignment of surface phonons at Si(*hkk*) modified by Au submonolayers** — ●JULIAN PLAICKNER<sup>1</sup>, EUGEN SPEISER<sup>1</sup>, SANDHYA CHANDOLA<sup>1</sup>, NOBERT ESSER<sup>1</sup>, BENEDIKT HALBIG<sup>2</sup>, and JEAN GEURTS<sup>2</sup> — <sup>1</sup>Leibniz-Institut für Analytische Wissenschaften-ISAS- e.V. Schwarzschildstrasse 8, 12489 Berlin, Germany — <sup>2</sup>Universität Würzburg, Physikalisches Institut, Experimentelle Physik 3 Am Hubland, 97074 Würzburg, Germany

Raman spectroscopy is an extremely sensitive tool for analyzing vibration modes of ordered (sub)monolayers of metal adatoms on semiconductor surfaces, which are typical systems for electron correlation effects. We report on the in situ UHV Raman analysis of self-organized Au submonolayers on nominal Si(111) surfaces, as well as on vicinal Si(553), Si(775), and Si(557). For the two-dimensional Au-( $\sqrt{3} \times \sqrt{3}$ ) and the one-dimensional Au-( $5 \times 2$ ) reconstructions, several specific Raman peaks in the spectral range below 200 cm<sup>-1</sup>

are assigned to Au-dominated vibrational modes, while Si-step-edge vibrational modes around 400 cm<sup>-1</sup> are fingerprints of the substrate orientation.

O 95.9 Fri 12:30 H14

**Tb induced surface structures on Si(110)** — ●STEPHAN APPELFELLER and MARIO DÄHNE — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Metallic rare earth silicide nanostructures are known to form by deposition of rare earth elements on clean Si substrates and annealing. The growth of nanowires is observed on Si(001) substrates due to anisotropic strain and on Si(*hkk*) substrates due to steps disrupting the two-dimensional film growth found on Si(111) substrates. Such rare earth silicide nanowires are not only interesting for studying the unique one-dimensional physics, but are also promising for future applications since they consist of the metallic bulk silicides, possibly allowing their passivation by capping without strong changes of their properties.

Here, the growth of Tb induced surface structures on the Si(110) surface is studied. Using scanning tunneling microscopy, single domain growth of Tb silicide structures with very high aspect ratios, i.e. of Tb silicide nanowires, is observed even on planar substrates due to its structural anisotropy. Furthermore, scanning tunneling spectroscopy clearly shows that these nanowires have a finite density of states at the Fermi level. In contrast, the wetting layer, which accompanies the nanowires formation, is characterized by a small band gap. This wetting layer is also studied using low energy electron diffraction revealing the formation of two domains.

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O 95.10 Fri 12:45 H14

**Charge density wave melting in one-dimensional wires with femtosecond sub-gap excitation** — ●MARIANA CHÁVEZ-CERVANTES, GABRIEL E. TOPP, SVEN AESCHLIMANN, RĂZVAN KRAUSE, SHUNSUKE A. SATO, MICHAEL A. SENTEF, and ISABELLA GIERZ — Max Planck Institute for the Structure and Dynamics of Matter

Charge density waves (CDWs) are symmetry-broken ground states that commonly occur in low-dimensional metals due to strong electron-electron and /or electron-phonon coupling. The non-equilibrium carrier distribution established via photodoping with femtosecond laser pulses readily quenches these ground states and induces an ultra-fast insulator-to-metal phase transition. To date, CDW melting has been mainly investigated in the single-photon and tunneling regimes, while the intermediate multi-photon regime has received little attention. Here we excite one-dimensional indium wires with a CDW gap of 300 meV with mid-infrared pulses at 190 meV with MV/cm field strength and probe the transient electronic structure with time- and angle-resolved photoemission spectroscopy (tr-ARPES). We find that the CDW gap is filled on a timescale short compared to our temporal resolution of 300 fs and that the phase transition is completed within 1 ps. Supported by a minimal theoretical model we attribute our findings to multi-photon absorption across the CDW gap.