O 18: Poster Monday: Nanostructures

Time: Monday 17:45–20:00 Location: Poster F

O 18.1 Mon 17:45 Poster F

Theoretical investigation of H adsorption at the Si(557)-Au surface — •Ferdinand Ziese, Kirs Holtgrewe, Christof Dues, and Simone Sanna — Justus-Liebig-Universität Giessen, Institut für Theoretische Physik Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Vicinal Si(111)-Au surfaces feature single or double atomic Au chains on each terrace of the stepped Si surface [1]. The metallic wires are electronically decoupled from the substrate and represent quasi 1D nanoobjects. In order to tune the wire metallicity, different atoms and molecules can be adsorbed on the system [2]. In this work, we investigate the adsorption atomic hydrogen at the Si(557)-Au surface within density functional theory. In a first step, the favorable adsorption site is determined as a function of the H coverage by means of potential energy surface calculations. While H adsorbs on the Si step edge on pristine surfaces, the favored site for the secondary H adsorption is on top of the so-called rest atom. Band structure calculations reveal that H acts as an electron donor, influencing the electronic states related to the adsorption sites. For an H coverage corresponding to two H atoms per (5x2) surface unit cell, we predict the formation of an electronic band gap at the Fermi energy and a metal-to-insulator transition.

[1] N. J. Crain et al., Phys. Rev. B 69, 125401 (2004)

[2] Z. Mamyev et al., Phys. Rev. Mat. 2, 066002 (2018)

O 18.2 Mon 17:45 Poster F

Theoretical investigation of the Au-induced Si(111) surface reconstruction — •Felix Bernhardt, Kris Holtgrewe, Christof Dues, and Simone Sanna — Justus-Liebig-Universität Giessen

The Au-induced reconstruction of the Si(111) surface is one of the most intensively investigated nanostructured systems. It features quasi one-dimensional (1D) chain structures, which are prototypical 1D metals on a 2D semiconducting surface. The debate on the structural model of the Au wires has been periodically reignited, with the theoretical models proposed by Erwin, Barke and Himpsel [1], Abukawa and Nishigaya [2], as well as Kwon and Kang [3], marking the cornerstones of a long investigation process. Although the Kwong-Kang model is currently accepted, there have been several attempts to refine the structure, e.g., by surface x-ray diffraction [4]. A structural modification has been proposed recently by the Wollschläger group in Osnabrück. In this work, we test different structural modifications proposed by the experiment within density functional theory. Thereby we analyze the bond lengths as well as the energetics of the relaxed structural models within different computational schemes. The calculations reveal that the proposed modifications do not lead to a new structural model, but rather relax to the Kwong-Kang structure. [1] S. C. Erwin et al., Phys. Rev. B 80, 155409 (2009) [2] Abukawa et al., Phys. Rev. Lett. 110, 036102 (2013) [3] S.-W. Kwon et al., Phys. Rev. Lett. 113, 086101 (2014) [4] T. Shirasawa et al., Phys. Rev. Lett. 113, 165501 (2014)

O 18.3 Mon 17:45 Poster F

First-principles investigation of the vibrational properties of rare-earth silicides on the Si(111) surface — •Vincent Maximilian Wettig, Kris Holtgrewe, Christof Dues, and Simone Sanna — Justus-Liebig-Universität Gießen, Gießen, Hessen

The investigation of the vibrational properties has recently become one of the most appealing tools for surface analysis. As Raman frequencies and selection rules are strongly related to the surface structure, they represent reliable criteria to identify, validate or rule out competing structural models [1].

In this work, we model from first principles the vibrational properties of rare-earth silicide monolayer structures deposited on Si(111) surfaces. As the resulting metal/semiconductor interface is characterized by an extraordinarily low Schottky-barrier height (0.3*0.4 eV on n-type substrates), the silicide nanostructures are both of technological and academic interest.

Employing previously proposed structural models based on the hexagonal DySi2 lattice [2], we demonstrate the existence of surface localized phonon modes of different symmetry in the frequency range between 25 and 500 cm-1 for the investigated dysprosium and terbium silicides. The rare earth atom has a minor influence on the calculated frequencies, which is attributed to the atomic mass difference.

[1] B. Halbig et al., Phys. Rev. B 97, 035412 (2018)

[2] S. Sanna et al., Phys. Rev. B 93, 195407 (2016)

O 18.4 Mon 17:45 Poster F

Au atomic wires on Si(hhk) substrates: Recent advances from experiment and theory — •Simone Sanna[1], Zamin Mamiyev[2], Christoph Tegenkamp[3], and Herbert Pfnür[2] — [1]Justus-Liebig-Universität Gießen — [2]Leibniz Universität Hannover — [3]Technische Universität Chemnitz

The investigation of substrate-supported quasi-1D atomic wires flourished in the last decade, owing to recent advances in experimental techniques for surface analysis, and fueled by the growing demand for outstanding materials. While many 1D properties are not spoiled by structural embedding, the coupling to the environment allows modifying physical properties, e.g., the wire metallicity. In this respect, Au wires grown on vicinal Si(111) surfaces are an ideal playground, as the miscut controls the wire width (single or double atomic rows) and the interwire distance. In this contribution, we report on theoretical and experimental studies recently performed to explore the coupling of Au wires on Si(hhk) surfaces with the environment. Adsorption of H and O is found to affect differently single and double Au wires [1]. The coupling of the wires to higher dimensions through the substrate results in the breakdown of the nearly-free electron gas model [2]. Thus, the wires are more appropriately described as extremely anisotropic 2D objects than as purely 1D.

[1] Z. Mamyev et al., Phys. Rev. Mat. 2, 066002 (2018). [2] S. Sanna et al., J. Phys. Chem. C 122, 25580 (2018). [3] Z. Mamyev et al., Phys. Rev. B, submitted.

O 18.5 Mon 17:45 Poster F

Multi-pulse excitation of one-dimensional nanowires at surfaces — •Nils Häusser, Jan Gerrit Horstmann, Hannes Böckmann, and Claus Ropers — IV. Physical Institute, University of Göttingen, Friedrich-Hund-Platz 1, Germany

Steering the making and breaking of bonds in solid-state phase transitions by intense light fields is one of the ultimate goals of ultrafast condensed matter physics. Multi-pulse [1] and resonant [2] optical excitation schemes promise coherent control over structural phase transitions in solids and at surfaces on their inherent time scale. Here, we explore the potential of multi-pulse excitation for inducing and controlling structural phase transitions in low-dimensional materials. Starting with a two-pulse scheme, we investigate and control the structural phase transition in In-nanowires on Si(111) [3]. We find that the transition is governed by the dynamics of only two structural modes, making indium on silicon a model system to study the feasibility of more complex and tailored excitation schemes.

[1] A. M. Weiner et al., Science 247, 1317-1319 (1990). [2] M. Rini et al., Nature 449, 72-74 (2007). [3] T. Frigge et al., Nature 544, 207-211 (2017).

O 18.6 Mon 17:45 Poster F

Simulating organic functionalization of Si(553)-Au — •Conor Hogan[1], Svetlana Suchkova[2], Friedhelm Bechstedt[3], Eugen Speiser[2], Sandhya Chandola[2], and Norbert Esser[2] — [1]Istituto di Struttura della Materia-CNR (ISM-CNR), Rome, Italy — [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V. Berlin — [3]Friedrich-Schiller-Universität Jena

Stepped gold-stabilized Si(553) surfaces offer much potential for self-organized assembly of one- and two-dimensional nanostructured arrays of organic molecules [1]. Regular atomic chains of Au and Si on the surface, running parallel to the step edges, act as natural templates for ordered organic functionalization. Strong covalent bonding to the semiconductor substrate determines that layer formation is controlled by the local surface reactivity. In this theoretical study we investigate the adsorption of various simple organic molecules with different functional groups on Si(553)-Au [2]. In particular we investigate the role of the functional group on the final geometry and electronic structure and show that hydrogen co-doping offers a means to tune the local reactivity [3].

[1] S. Suchkova, C. Hogan, F. Bechstedt, E. Speiser, N. Esser, Phys. Rev. B 97, 045417 (2018). [2] C. Hogan, S. Suchkova, F. Bechstedt, E. Speiser, S. Chandola, N. Esser, submitted. [3] C. Hogan, E. Speiser, S. Chandola, S. Suchkova, J. Aulbach, J. Schäfer, S. Meyer, R. Claessen,

and N. Esser, Phys. Rev. Lett. 120, 166801 (2018).

O 18.7 Mon 17:45 Poster F

Highly Ordered Metallic Phase of Indium on SiC(0001) — Maximilian Bauernfeind, •Jonas Erhardt, Jörg Schäfer, and Ralph Claessen — Physikalisches Institut and Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Germany

For the monolayer growth of two-dimensional topological insulators (2D-TIs) on the insulating SiC(0001) substrate, the strong interaction between the deposited layer and the substrate dangling bonds (DBs) plays a pivotal role and drastically affects the electronic structure of the system. Especially 2D-TIs with fragile topology, e.g. quasi-freestanding stanene, require a passivated substrate to cancel out such interactions that are detrimental for the topological properties [1]. Indium with its three valence electrons is such a passivation candidate and leads to metallic or insulating phases on various semiconducting surfaces. Here we report first results of a highly ordered indium phase on SiC(0001). Scanning tunneling microscopy (STM) reveals a Kagome-like superstructure with a lattice constant of approximately 2.1 nm tentatively assigned as a $(4\sqrt{3}\times4\sqrt{3})$R30° reconstruction. Additionally, scanning tunneling and angle-resolved photoelectron spectroscopy (STS and ARPES) show a band structure distinct from pristine SiC and reveal a metallic character with a pronounced electron pocket, indicative of a 2D electron gas. Interestingly, despite the large unit cell observed in STM and low-energy electron diffraction, the corresponding Brillouin zone is not effective in the ARPES band structure.

[1] D. Di Sante et al., arXiv:1807.09006 (2018)

O 18.8 Mon 17:45 Poster F

Sn nanowires on a vicinal Si(111) surface — •Monika Jäger[1], Herbert Pfnür[1], Mauro Franciulli[2], Andrew Weber[2], Jan-Hugo Dil[2], and Christoph Tegenkamp[1,3] — [1]Leibniz Universität Hannover, Germany — [2]Swiss Light Source, Villigen, Switzerland — [3]TU Chemnitz, Germany

The α-Sn phase on Si(111) is a prototype system for a two-dimensional Mott phase. Recently, the low temperature phase was investigated by means of spin-resolved ARPES showing that the formation of the row-wise collinear antiferromagnetically spin-ordering is accompanied by a small Rashba-splitting of the highest occupied Mott state [1].

In order to study the influence of confinement towards the Mott state we studied the growth of Sn-nanowires on vicinal Si(111) by means of STM and ARPES. Depending on the Sn coverage, three different phases were identified. At low coverages, the surface structure of Si(557) is preserved comprising 3 nm wide α-Sn stripes. They exhibit a metallic surface state in ARPES at low temperatures possibly due to doping of the Mott state via step edges. Similar observations of metallic QP states were reported for hole doped α-Sn/Si(111) [2]. Further increase of the coverage to 0.5 ML leads to a refacetting of the surface exhibiting locally a (223) orientation. The wider (111) terraces reveal both $(\sqrt{3}\times\sqrt{3})$ and $(2\sqrt{3}\times2\sqrt{3})$ Sn reconstructions, the latter is well known for 0.3-1.2 ML Sn/Si(111). For higher coverages (>0.7 ML), step bunching sets in resulting in wide $(2\sqrt{3}\times2\sqrt{3})$-domains.

[1] M. Jäger et al., PRB **98**, 165422, (2018).
[2] F. Ming et al., PRL **119**, 266802, (2017).

O 18.9 Mon 17:45 Poster F

Forming and contacting chains of Fe and Co nanoclusters for four-probe transport measurements — •Oleg Kurnosikov[1] and Kongyi Li[2] — [1]Eindhoven University of Technology, Eindhoven, The Netherlands — [2]QuTech, Delft University of Technology, Delft, The Netherlands

Electron transport along a chain of nanoclusters can be governed by a single-electron charge, spin or quantum phenomena as soon the size of the nanoclusters is in the order of several or tens nanometers. To fabricate such system aiming at spin transport we arrange the chains of small Fe and Co nanoclusters on an ultra-thin AlOx layer. Within our approach, the thin oxide layer decouples the electronic states of the nanoclusters from a conductive substrate. Iron and cobalt nanoclusters were obtained by MBE growth at controlled temperature in UHV. The arrangement of the clusters in chains is achieved by exploiting a preferable nucleation along the structural defects of AlOx or, alternatively, by relocation of the individual nanoclusters with the STM tip. However, a direct contacting the chains of nanoclusters for current transport measurements with the four-probes method is not trivial since the contacting process becomes destructive on this scale both for the clusters and thin alumina layer. To solve the problem of 4-probe contacting to the chain we introduced auxiliary gold islands of bigger size mediating the contacts with four probes. Various ways of formation of the gold islands providing the reliable contacts have been tried.

O 18.10 Mon 17:45 Poster F

Surface dependent analysis of freestanding GaAs-nanowires — •Andreas Nägelein[1], Juliane Koch[1], Matthias Steidl[1], Stefan Korte[2], Bert Voigtländer[2], Peter Kleinschmidt[1], and Thomas Hannappel[1] — [1]Institute of Physics, TU Ilmenau, 98693 Ilmenau, Germany — [2]Peter Grünberg Institut (PGI-3,) Forschungszentrum Jülich, 52425 Jülich, Germany

Nanostructures e.g. III-V nanowires (NW) are known as promising candidates for optoelectronic applications. In this work we investigate single, freestanding "vapor liquid solid" (VLS) grown GaAs-NWs by a multi-tip scanning tunneling microscope (MT-STM). Here, four-point probe measurements are performed non-destructively by contacting three tips at the nanowire and using the substrate as a fourth contact. Besides the investigation of doping profiles, a comparison between nanowires prior to and after oxidation was carried out. The resistance slope in the intrinsic part of the NW increased drastically with oxidation. In contrast to doped NW-parts where the charge carrier transport mainly takes place in the center of a NW, a conductive channel does not exist for intrinsic NWs. Besides contamination-induced band bending, the conductivity is also affected by the surface states themselves. Since oxidation changes the surface states and thereby the space charge layer, we consider a changed surface conductivity of the intrinsic nanowire segment as a likely explanation of its increased resistance after exposure to ambient atmosphere.

O 18.11 Mon 17:45 Poster F

Tailor-made *meso to macro* porous CuNi films by electrodeposition: synthesis and application — •Jin Zhang[1,2], Jordi Sort[2,3], and Eva Pellicer[2] — [1]State Key laboratory of Solidification Processing, Center of Advanced Lubrication and Seal Materials, Northwestern Polytechnical University, Xi'an, Shaanxi, 710072, P. R. China — [2]Departament de Física, Universitat Autònoma de Barcelona, E-08193 Bellaterra, Spain — [3]ICREA, Pg. Lluís Companys 23, E-08010 Barcelona, Spain

Porous films with interconnected pores of different dimensions are attractive in many fields like catalysis, gas adsorption, or energy storage, etc. Template-assisted electrodeposition (ED) is very effective to fabricate porous films since meso- to macro-scale pores can be obtained by changing templates. In this talk, the production of macroporous CuNi films by hydrogen bubble-assisted ED is demonstrated. The synthetic approach results in porous films with highly interconnected nanodendritic walls[1]. Moreover, P123 tri-block copolymer is used for the ED of mesoporous CuNi films. Pores between 5 nm and 20 nm and dissimilar space arrangements are obtained depending on the parameters[2]. These meso- to macro-porous CuNi films exhibit enhanced electrocatalytic activity towards hydrogen evolution reaction. From a technological point of view, they can also be used as scaffold to host other functional materials that could bring hydrophilic/hydrophobic properties, electrical insulation or even enhanced mechanical performance.

[1] Nanoscale 2014, 6, 12490. [2] ACS Appl. Mater. Interfaces 2018, 10, 14877