HL 73: Semiconductor Surfaces (joint session O/HL)

Time: Thursday 15:00–17:30 Location: REC C 213

HL 73.1 Thu 15:00 REC C 213

Time-resolved reflection anisotropy spectroscopy reveals the impact of surface non-idealities for water adsorption on GaP — •Matthias M. May[1], Helena Stange[1], Jonas Weinrich[2], Thomas Hannappel[3], and Oliver Supplie[3,4] — [1]Helmholtz-Zentrum Berlin, Germany — [2]Ferdinand-Braun-Institut, Berlin, Germany — [3]Technische Universität Ilmenau, Germany — [4]Humboldt-Universität zu Berlin, Germany

The initial interaction of water with semiconductor surfaces typically leads to surface chemical reactions, which determine the electronic structure of the solid–liquid interface as well as stability against corrosion. Access to this interface to reveal the nature of the interaction is, however, challenging. Here, we study gallium phosphide-based (100) surfaces exposed to H_2O by means of time-resolved reflection anisotropy spectroscopy during water adsorption in vacuum [1]. We show that the introduction of imperfections in the form of surface steps via substrate off-cut variation or trace contaminants not only changes the dynamics of the interaction, but also its qualitative nature. While the clean surface without steps does not show any presence of oxygen after several 10 kL of exposure at room temperature, this changes with the introduction of trace carbon or a substrate off-cut. The decay rate of the surface optical anisotropy allows us to estimate activation energies of the surface reactions. Our findings emphasise the challenges for the comparability of experiments with idealised electronic structure models.

[1] May et al., *SciPost Physics* **6**, 058 (2019).

HL 73.2 Thu 15:15 REC C 213

Ion-Induced Surface Nanostructures of Germanium(001) — •Ricardo de Schultz, Denise Erb, and Stefan Facsko — Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden, Germany

Ion beam irradiation can lead to various self-organized surface nanopatterns depending on the irradiation conditions and the sample material. In this case, the surface patterns of Ge(001), which evolve during high-fluence 1 keV ion irradiation with Ar^+ ions at elevated temperatures, have been studied. Whereas at room temperature the semiconductor surface would become amorphous during ion irradiation, high temperatures enhance the diffusion so that bulk vacancies and interstitials can recombine before the next ion hits the same surface region. Thus the surface stays crystalline. This results in a biased surface diffusion because of the Ehrlich-Schwoebel barrier at step edges and kinks.

The periodic surface patterns that emerge on Ge(001) reflect the four-fold symmetry of the crystalline surface. These patterns consist of a checkerboard of inward and outward oriented pyramids. For normal ion incidence their bases are square and oriented along the <100> crystal direction. For two different azimuthal ion incidence angles - along <110> and <100> - the emerging patterns have been examined for different polar incidence angles and compared to simulations. These indicate that the height gradient dependent sputter erosion plays an important role during pattern formation.

HL 73.3 Thu 15:30 REC C 213

Structural and Electronic Properties of the FeSi(110) Surface — •Biao Yang[1], Martin Uphoff[1], Yi-Qi Zhang[1], Joachim Reichert[1], Ari P. Seitsonen[2], Andreas Bauer[3], Christian Pfleiderer[3], and Johannes V. Barth[1] — [1]Physics Department E20, Technical University of Munich, D-85748 Garching, Germany — [2]Département de Chimie, École Normale Supréieure, 24 rue Lhomond, F-75005 Paris, France — [3]Physics Department E51, Technical University of Munich, D-85748 Garching, Germany

Iron silicide (FeSi) is a fascinating material which has attracted numerous research efforts for decades.[1] It has B20 crystal structure featuring cubic unit cell without an inversion center. To gain insight into the unusual surface properties of this system, we successfully prepare the atomically flat FeSi(110) surface with the Ar ion sputtering and annealing treatment. By scanning tunneling microscopy (STM), we clearly resolve a step-terrace topography and the details of the atomic lattice. The atomically resolved STM images and DFT calculations give strong indications for the surface termination, where the topmost comprises of one Fe and one Si atom. Furthermore, a small energy gap of 80 meV close to the Fermi level is derived by scanning tunneling spectroscopy (STS). Intriguingly, two in-gap states are identified for the first time. References 1. V. Jaccarino, G. K. Wertheim, J. H. Wernick, L. R. Walker, S. Arajs. Phys. Rev. 1967, 160, 476.

HL 73.4 Thu 15:45 REC C 213

Detection of stress hormone cortisol in saliva using silicon nanowire field effect transistors with a portable measurement system — •Stephanie Klinghammer[1], Nadia Licciardello[1], Tetiana Voitsekhivska[2], Clemens Kirschbaum[3], Larysa Baraban[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [3]3Department of Psychology, TU Dresden, 01062 Dresden Germany

The accurate and rapid detection of various targets from patients on portable point-of-care devices is attracting great attention in bio- and nanotechnology for more than a decade [1]. Here, we demonstrate a portable, label-free and real-time sensing platform based on silicon nanowire field effect transistors which is capable for detection of several small molecules [2]. We particularly focus on the sensitive recognition of the stress hormone cortisol by using aptamers as receptors in order to allow high sensitive screenings in physiological conditions. We show the working principle by determination of cortisol levels in saliva of volunteers and compared to levels obtained with conventional ELISA method.

References: [1] Patolsky F, Zheng G, Lieber CM. 2006. Nanomed. 1(1):51*65 [2] Voitsekhivska T, Suthau E, Wolter K-J. 2014. in IEEE. 173-178

Invited Talk HL 73.5 Thu 16:00 REC C 213

Coupling of electronic and atomic degrees of freedom in surface-stabilized quasi-1D systems — •Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn

Minute structural changes may lead to drastic modifications of the electronic properties of quasi-1D systems, while, on the other hand, an electronic charge redistribution, induced, e.g., by optical excitations or surface vibrations may induce pronounced structural modifications in such systems. This is illustrated in my talk using two prominent examples: (i) Localized photoholes at the Brillouin zone boundary of the In/Si(111)(8x2) nanowire system are shown to drive an ultrafast (8x2) $\longrightarrow$ (4x1) phase transitions that is accompanied by the formation of metallic In-In bonds along the wire direction [1,2]. (ii) A Si $sp^3 \longrightarrow sp^2+p$ rehybridization accompanied by a lateral surface charge transfer is demonstrated to destabilize the Si(553)-Au spin chains [3] with respect to a diamagnetic surface ground state that complies with electron counting heuristics [4]. Thermal excitation leads to soft Au chain vibrations that alter transiently the Au electron affinity and eventually the hybridization of the Si step edge atoms.

[1] T Frigge et al., Nature 544, 207 (2017).
[2] CW Nicholson et al., Science 362, 821 (2018).
[3] SC Erwin, FJ Himpsel, Nat. Commun. 1, 58 (2010).
[4] C Braun et al., PRB 98, 121402(R) (2018).

HL 73.6 Thu 16:30 REC C 213

Determining surface phase diagrams including anharmonic effects — •Yuanyuan Zhou, Matthias Scheffler, and Luca M. Ghringhelli — Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin-Dahlem, Germany

A prerequisite for analyzing and understanding the electronic properties and the function of surfaces is the detailed knowledge of their structure under realistic conditions. We have developed a replica-exchange grand-canonical (REGC) algorithm that enables the unbiased calculation of pressure-temperature phase diagrams of surfaces or clusters in reactive atmospheres including anharmonic effects. [1] Moreover, the multi-canonical sampling yields the temperature-pressure dependence (map) of all equilibrium observables that can be measured within the given model Hamiltonian. For instance, structural parameters such as the radial distribution function, or the HOMO-LUMO gap. This allows for rational design, where *operando* condition are taking fully

into account. Our approach is demonstrated by studying Si clusters and the Si(100) surface in a hydrogen atmosphere, by coupling REGC with *ab initio* molecular dynamics. All interactions are described at the density-functional-theory level, with the Perdew-Burke-Ernzerhof gradient-corrected exchange-correlation functional. In particular, we show how to determine *observable structures* at finite temperature and pressure, i.e., obtained by ensemble averaging the sampled structures. [1] Y. Zhou, M. Scheffler, and L. M. Ghringhelli, Phys. Rev. B. 100, 174106 (2019).

HL 73.7 Thu 16:45 REC C 213

Doping-induced metal-insulator transition in Au atomic wires — •Zamin Mamiyev[1], Simone Sanna[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Appelstrasse 2 Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany — [2]Institut für Theoretische Physik, Justus-Liebig- Universität Gießen

Close coupling between structural and electronic parameters has been demonstrated in the past for arrays of quasi one-dimensional Au chains on Si surfaces. Here we employ plasmon spectroscopy and LEED to study electronic and structural modifications as a result of surplus Au concentrations, x, starting at 0.48 ML on Si(553) and at 0.65 ML on Si(111). For the Si(111)-Au surface an abrupt metal-insulator transition (MIT) was observed by adding more than 0.05 ML Au. In contrast, the Si(553)-Au surface shows a rather gradual decrease of plasmon frequency up to x= 0.1 ML. Moreover, self-doping with Au on Si(553)-Au improves the chain quality up to x=0.03 ML, resulting also in an increase of plasmon intensity. Further addition of Au at room temperature leads to a vanishing plasmon frequency, coupled with the disappearance of the $\times 2$ periodicity. By annealing the doped samples at 630°C the Au atoms form small clusters with $(\sqrt{3} \times \sqrt{3})$R30° symmetry, while the metallicity of the Au chains is fully recovered, but the structural imperfections in the chains as well. The appearance of $\sqrt{3}$-order indicates local restructuring into larger terraces and their spatial separation from the Au-chains. This proves that not only the amount of dopant but also its distribution is important for reversible MIT on such surfaces. These findings were corroborated by DFT calculations.

HL 73.8 Thu 17:00 REC C 213

Selective Excitation of Amplitude Modes Driving the In/Si(111) Peierls Transition — •Hannes Böckmann-Clemens, Jan Gerrit Horstmann, and Claus Ropers — 4th Physical Institute, Solids and Nanostructures, University of Göttingen, Göttingen 37077,Germany

The use of laser pulses to actively steer a system along the transition pathway from a reactant towards a desired product state is a fundamental scheme in the field of femtochemistry. Transferring this concept to solid-state surface systems requires the ultrafast manipulation of coherent phonons, associated with the reaction coordinate. Here, we demonstrate the mode-selective vibrational control over the Peierls metal-to-insulator phase transition of In/Si(111) by means of tailored pulse sequences. We explore the potential energy surface spanned by the amplitude modes of the system via selection of specific pathways along the transition path. We identify two essential modes, identify their separate roles in controlling the transition, and carry out experiments with mode-selective excitation.

HL 73.9 Thu 17:15 REC C 213

Novel electronic junctions in an atomic wire array: metallic states, charge density waves and solitonic excitations — •Abdus Samad Razzaq[1], Sun Kyu Song[2], Han Woong Yeom[2], and Stefan Wippermann[1] — [1]Max-Planck-Institut für Eisenforschung, Germany — [2]Pohang University, South Korea

The Si(111)-(4x1)In atomic wire array is an extremely popular model for one-dimensional (1D) 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 coexist and form novel types of electronic junctions between the metallic (4x1) phase and the insulating CDW-ordered (8x2) phase. Furthermore, the CDW phase is 4-fold degenerate, giving rise to solitonic excitations of the CDW, that take the form of phase boundaries between different CDW ground states. Combining scanning tunnelling microscopy (STM) and ab initio molecular dynamics (AIMD) calculations, we explore the microscopic structures of interfaces between distinct electronic phases at the atomic scale. These models enable insights into soliton propagation and soliton-mediated charge transport. Financial support from the German Research Foundation (DFG), grant no. FOR1700, and BMBF NanoMatFutur, grant no. 13N12972, is gratefully acknowledged.