O 2: Heterostructures, interfaces and surfaces (joint session HL/O)

Time: Monday 9:30–13:00 Location: POT 151

O 2.1 Mon 9:30 POT 151

Determining the band alignment of copper oxide-gallium oxide heterostructures — •Sebastian Leonard Benz, Martin Becker, Angelika Polity, Sangam Chatterjee, and Peter Jens Klar — Institute for Experimental Physics I and Center for Materials Research (LaMa), Justus Liebig University Giessen, Germany

The copper oxides cuprite (Cu_2O) and tenorite (CuO) are ideal candidates for solar cells as they promise high conversion efficiencies according to the Shockley-Queisser limit[1]. However, both cannot readily be doped n-type, hampering charge-carrier extraction of the photoexcited electron-hole pairs. The combination of the copper oxides with gallium sesquioxide is considered an excellent heterojunction system for overcoming this challenge. In such a pn junction, the p-type copper oxide layer will act as absorber and the transparent n-type gallium sesquioxide as window layer. In these devices, the band alignment at the internal interface is crucial for the device performance. Here, we study the band alignments of different copper oxide-gallium sesquioxide heterostructures by X-ray photoelectron spectroscopy. Within the experimental margin of error, Cu_2O-α-Ga_2O_3 appears to offer the most favourable band alignment for photovoltaic applications.

[1] William Shockley and Hans J. Queisser (March 1961). Journal of Applied Physics. 32 (3): 510*519.

O 2.2 Mon 9:45 POT 151

Nanometer Scale Characterization of Al/TiOx/SiOx Electron Selective Passivating Contacts Utilizing Advanced TEM Methods — •Christoph Flathmann[1], Tobias Meyer[1], Valeriya Titova[2,3], Jan Schmidt[2,3], and Michael Seibt[1] — [1]University of Goettingen, IV. Physical Institute, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute for Solar Energy Research Hamelin (ISFH), Emmerthal, Am Ohrberg 1, 31860, Germany — [3]Institute of Solid-State Physics, Leibniz University Hannover, Hannover, Appelstraße 2, 30167, Germany

One promising possibility to further increase photovoltaic efficiency and to enable new solar cell designs is the development of carrier selective passivating contacts. A particularly interesting electron selective passivating contact consists of an n-type crystalline Si base with tunnel silicon oxide (SiO_x), atomic layer deposited sub-stoichiometric titanium oxide (TiO_x) and aluminum as a rear contact. It is commonly assumed that SiO_x ensures high chemical interface passivation, whilst oxygen vacancies in the TiO_x result in an increased open circuit voltage. However, the detailed interplay of structure, composition and electrical properties is not entirely understood yet. We, therefore, apply various STEM techniques, such as EDX, EELS and 4D-STEM, to characterize such contacts for differently treated samples. The analytical methods show strong interdiffusion at the interfaces; in particular, intermixing of Al and TiO_x appears to be important for contact quality. Furthermore, the capabilities of medium resolution 4D-STEM to elucidate properties of such interfaces are explored.

O 2.3 Mon 10:00 POT 151

direct insight into the structure-property relation of interfaces from first-principles crystal structure prediction — •Lin Sun[1], Miguel A. L. Marques[2,3], and Silvana Botti[1,3] — [1]Institut für Festkörpertheorie und Optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut für Physik - Martin-Luther-Universität Halle, D-06099 Halle, Germany — [3]European Theoretical Spectroscopy Facility

In this work we develop an efficient and accurate computational scheme aimed at a full understanding of heterogeneous materials. Our approach is a variant of the minima-hopping method for global crystal structure prediction. Specifically, we implement a constraint library and we enable variations of the atomic density in proximity to the interface. DFT and DFTB calculations supply necessary energy and forces to the minima-hopping algorithm. With this method, we find a rich polymorphism in the reconstructions of tilt boundaries in polycrystalline silicon, with recurring bonding patterns that we classify in increasing energetic order. In several cases, we succeed in identifying atomic arrangements that are significantly more stable than previously predicted structures, while in other cases we show that the algorithm can recover, without experimental input, geometries that had been built by hand to match experimental data. We extend then the calculations to other group IV elements, and compare lowest energy reconstructions of C, Si, Ge and Sn grain boundaries. Finally, a clear relation between bonding patterns and electrically active interface states is unveiled and discussed.

O 2.4 Mon 10:15 POT 151

Effect of KF and RbF post-deposition treatments on the electronic structure of the CdS/Cu(In,Ga)Se2 interface in thin-film solar cells investigated by Kelvin Probe and Photoelectron Yield Spectroscopy — •Marin Rusu[1], Tim Kodalle[2], Leo Choubrac[1], Sergiu Levcenco[1], Nicolas Barreau[3], Christian Kaufmann[2], Rutger Schlatmann[2], and Thomas Unold[1] — [1]Struktur und Dynamik von Energiematerialien, Helmholtz-Zentrum Berlin für Materialien und Energie, Lise-Meitner Campus, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]PVcomB, Helmholtz-Zentrum Berlin für Materialien und Energie, Schwarzschildstr. 3, 12489 Berlin, Germany — [3]Institut des Matériaux Jean Rouxel (IMN)-UMR6502, Université de Nantes, 2 rue de la Haussinière, 44322 Nantes Cedex 3, France

We investigate the impact of potassium fluoride (KF) and rubidium fluoride (RbF) post-deposition treatments on electronic features of the Cu(In,Ga)Se2 (CIGSe) layer and CdS/CIGSe interface in a sequential time-dependent CdS thickness evolvement over the chemical bath deposition (CBD) process. Kelvin Probe and Photoelectron Yield Spectroscopy methods have been employed. Although we observe similarities with the reported data, we observe additional distinct features. We find that after an initial CBD stage the valence band maximum of the CIGSe surface is significantly shifted (by 180-620 mV) towards the Fermi level. In addition, K and Rb act as compensating dopants in CdS. Energy level diagrams are proposed and discussed.

O 2.5 Mon 10:30 POT 151

Template-Guided Programmable Janus Heteronanostructure Arrays for Efficient Plasmonic Photocatalysis — •Zhiqiang Zeng, Rui Xu, Huaping Zhao, and Yong Lei — Technische Universität Ilmenau, 98693, Ilmenau, Germany.

Janus heteronanostructures (HNs), as an important class of anisotropic nanomaterials, could facilitate synergistic coupling of diverse functions inherited by their comprised nanocomponents. Nowadays, synthesizing deterministically targeted Janus HNs remains a challenge. Here, a general yet scalable technique is utilized to fabricate an array of programmable Janus HNs based on anodic aluminum oxide binary-pore templates. By designing and employing an overetching process to partially expose four-edges of one set of nanocomponents in a binary-pore template, selective deposition and interfacing of the other set of nanocomponents is successfully achieved along the exposed four-edges to form a densely packed array of Janus HNs on a large scale. In combination with an upgraded two-step anodization, the synthesis provides high degrees of freedom for both nanocomponents of the Janus HNs, including morphologies, compositions, dimensions, and interfacial junctions. Arrays of TiO2-Au and TiO2/Pt NPs-Au Janus HNs are designed, fabricated, and demonstrated about 2.2 times photocurrent density and 4.6 times H2 evolution rate of that obtained from their TiO2 counterparts.

30 min. break.

Invited Talk O 2.6 Mon 11:15 POT 151

Exciton-Polariton Topological Insulator — •Sebastian Klembt — Technische Physik, Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Topological insulators (TIs) constitute a striking example of materials in which topological invariants are manifested in robustness against perturbations. The most striking characteristic is the emergence of topological edge states at the interface between areas with distinct topological invariants. The observable physical effect is unidirectional, robust edge transport, immune to disorder or defects. TIs have at first been observed in the integer quantum Hall effect in fermionic systems of correlated electrons. However, during the past decade the concepts of topological physics have been introduced into numerous fields be-

yond condensed matter, including photonic systems. Recently, TIs were proposed in exciton-polariton systems organized as honeycomb lattices, under the influence of a magnetic field. Exciton-polaritons are the new eigenstate quasiparticles resulting from the strong coupling of quantum well excitons to light in an optical microcavity mode. Here, we demonstrate experimentally the first exciton-polariton TI and as such the first symbiotic light-matter TI. In polaritonic honeycomb lattices, we show the existence of a C = 2 Chern TI, manifesting in a chiral, topologically protected edge mode. Notably, due to the driven-dissipative nature of polaritons this is an open system, with a strong non-linearity still preserving the topological mode.

O 2.7 Mon 11:45 POT 151

Quantum spin Hall quantum point contacts — •Niccolo Traverso Ziani[1], Bjoern Trauzettel[2], Christoph Fleckenstein[2], Lorenzo Privitera[2], and Maura Sassetti[1] — [1]Università degli Studi di Genova, Genova, Italy — [2]Universitaet Wuerzburg, Wuerzburg, Deutschland

The edges of two-dimensional topological insulators are fashinating systems. In order to fully exploit their potential, gaps need to be induced. While superconducting gaps can be implemented, magnetic and interaction-related ones seem to be experimentally challenging. We propose a wide range of possibilities enabled by the gaps that can open when constrictions between helical edges[1] are created. Jackiw-Rebbi charges[2], Majorana bound states[3], parafermions[4] and Floquet bound states[5] are addressed.

[1] J. Strunz, J. Wiedenmann, C. Fleckenstein, L. Lunczer, W. Beugeling, V. L. Mueller, P. Shekhar, N. Traverso Ziani, S. Shamim, J. Kleinlein, H. Buhmann, B. Trauzettel, and L. W. Molenkamp, Nat. Phys. (2019).

[2] C. Fleckenstein, N. Traverso Ziani, and B. Trauzettel EPL (Europhysics Letters) 121, 57003 (2018).

[3] C. Fleckenstein, N. Traverso Ziani, and B. Trauzettel, in preparation

[4] C. Fleckenstein, N. Traverso Ziani, and B. Trauzettel, Phys. Rev. Lett. 122, 066801 (2019)

[5] C. Fleckenstein, N. Traverso Ziani, L. Privitera, M. Sassetti, and B. Trauzettel, arXiv:1908.11719

O 2.8 Mon 12:00 POT 151

Correlation of optical properties and interface morphology in type-II semiconductor heterostructures — •Luise Rost, Jannick Lehr, Milan Maradiya, Wolfgang Stolz, and Wolfram Heimbrodt — Department of Physics and Materials Sciences Center, Philipps-Universität Marburg, Germany

The (Ga,In)As/GaAs/Ga(As,Sb) material system is used for lasers operating over a wide spectral range in the infrared. To further optimize the design of such heterostructures, it is important to have deep understanding of the influence of the interface morphology and the charge carrier dynamic through the interface. Here (Ga,In)As/GaAs/Ga(As,Sb) type-II double quantum well heterostructures has been grown by metall-organic vapor phase epitaxy. A growth interruption procedure was used to intentionally modify the morphology of the internal interfaces. The heterostructures were investigated using continuous wave and time-resolved photoluminescence spectroscopy. A correlation was revealed between the interface morphology and optical and kinetic properties. AFM images of the as grown interface surfaces show substantially smoother interfaces both on vertical as well as lateral length scales. We will illustrate that for every used material there is a matching growth interruption time to further enhance the optical response of such a type-II heterostructure.

O 2.9 Mon 12:15 POT 151

First-principles study of the structural and electronic properties of the GaAsxP1-x surface — •Marsel Karmo and Erich Runge — TU ILmenau, Weimarer Str.32, 98693 ILmenau

GaAsP is a III-V semiconductor alloy, which forms crystals in zincblende structure. Due to its high electron mobility, it is an important material in optoelectronics, mainly for solar cells. For the latter, it is important to understand the surface relaxation and reconstruction in the P-rich MOVPE process. We use the Vienna Ab initio Simulation Package (VASP) to perform first-principles calculations to identify the composition-dependent surface reconstructions and bonding-sites for adsorbates.

O 2.10 Mon 12:30 POT 151

Copper iodide thin films: Dynamic AFM studies of local electrical properties — •Tillmann Stralka, Chang Yang, Holger von Wenckstern, and Marius Grundmann — Solid State Physics, Leipzig, Germany

The search for high-performance p-type transparent conductive materials has been a major challenge in decades [1]. Copper iodide (CuI) or alloys based on CuI [2] could offer a solution, since CuI does outperform all other known p-type TCMs, concerning transmittance in the visible spectrum as well as electrical conductivity at room temperature [3]. In this contribution polycrystalline CuI thin films grown by sputtering, are investigated. Hereby we try to understand the impact of grains and grain boundaries (GBs) on transport mechanisms. Topographic features as GBs lead to a depletion of majority charge carriers and even a localized inversion (two dimensional electron gas) within GBs [4]. To acquire morphological and electrical properties with a high spatial resolution we employ atomic force microscopy, which additionally offers different modes to characterize electrical properties (such as: capacitance, conductivity and work function). These measurements will be conducted and evaluated with a novel approach that offers voltage spectroscopy and localization of sub-nm sized objects at the same time and furthermore correlate topographic features with electrical properties.

[1] M. Grundmann et al., J.Phys.D.Apps.Phys., 49(213001), 2016 [2] T. Jun et al., Adv. Mater. 30(1706573), 2018 [3] C. Yang et al., PNAS 113(412929) [4] M. Kneiß et al., Adv. Mater. Interfaces, 5(6), 2018

O 2.11 Mon 12:45 POT 151

Stability and Tunneling Transport Properties of $NiSi_2$-Si Interfaces — •Florian Fuchs[1,2,3,4], Sibylle Gemming[2,3], and Jörg Schuster[1,2,3,4] — [1]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [2]Chemnitz University of Technology, Chemnitz, Germany — [3]Center for Advancing Electronics Dresden (cfaed), Dresden, Germany — [4]Forschungsfabrik Mikroelektronik, Berlin, Germany

Metal-semiconductor interfaces are of huge importance for applications and are considered for various modern device architectures. We study the interface between $NiSi_2$ and silicon on the basis of density functional theory. Different crystal orientations and strain states are investigated systematically. The energetically most favorable interface orientation is worked out, which can explain recent experimental observations [1]. Using atomistic quantum transport simulation, the tunneling transport through the interface is calculated [2]. The transport is related to underlying properties including the Schottky barrier height and the effective mass. This is done on the basis of the Wentzel-Kramers-Brillouin approximation, which can describe the tunneling transport reasonably well. Finally, the Schottky barrier height and its strain dependence is discussed in the context of the metal-induced gap states model.

[1] Khan et al., *Appl. Sci.* **9**, 3462 (2019)
[2] Fuchs et al., *J. Phys.: Condens. Matter* **31**, 355002 (2019)