HL 5: Heterostructures, interfaces and surfaces

Time: Monday 10:00–11:15 Location: POT 112

HL 5.1 Mon 10:00 POT 112

Time-resolved analysis of propagating exciton-polariton condensates in photonic potential landscapes. — •Christian G. Mayer, Philipp Gagel, Simon Betzold, Tristan H. Harder, Monika Emmerling, Adriana Wolf, Fauzia Jabeen, Sven Höfling, and Sebastian Klembt — Technische Physik, RCCM and Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg, Germany

Confining photons in a Fabry-Perot microcavity and coupling them strongly to excitons leads to the formation of hybrid matter-light particles named exciton-polaritons (polaritons). Owing to their bosonic statistics, they undergo a phase transition above a critical density to a dynamic condensate via stimulated scattering. Polaritons have quite long diffusion length compared to excitons because of their lower effective mass inherited by their photonic fraction. Propagation effects of a polariton condensate take place on a time scale of a few picoseconds and are caused by the repulsive potential facilitated by the matter fraction due to polariton-exciton and polariton-polariton interactions. By varying the light-matter composition of the polariton condensate, we investigate changes in the propagation properties such as velocity and length.

Using electron beam lithography, we spatially confine propagating polaritons in waveguides, as well as in resonator lattices supporting quantum valley Hall modes. Using a streak camera, the propagation of the polariton condensate is measured in a variety of confined structures and systems.

HL 5.2 Mon 10:15 POT 112

Tackling the band ordering problem for transport calculations in strained semiconductors: A k × p perspective — •Daniel Fritsch[1], Costanza L. Manganelli[2], Christian Merdon[1], and Patricio Farrell[1] — [1]Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstr. 39, 10117 Berlin, Germany — [2]IHP Leibniz-Institute for High Performance Microelectronics, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

A reliable determination of band energies in strained semiconductor heterostructures is indispensable for subsequent transport calculations. However, one crucial problem is presently hidden within the change in valence band ordering due to intrinsically occurring strain in semiconductor heterostructures, nanowires, or quantum dots.

In order to tackle this problem, we present a numerical algorithm based on the Bir-Pikus $\mathbf{k} \times \mathbf{p}$ Hamiltonian, that takes into account additional wavevector dependent properties, e.g. the effective mass tensor, to identify the nature of the valence bands. It provides the necessary connection between arbitrary strain profiles for semiconductor nanostructures calculated by means of a finite element method [1] and transport calculations employing a drift diffusion model [2].

The new algorithm is applied to example strain profiles, e.g. biaxial and uniaxial strain, and results are compared to earlier theoretical and experimental findings.

[1] GradientRobustMultiPhysics.jl (10.5281/zenodo.7217591).
[2] ChargeTransport.jl (10.5281/zenodo.7124161).

HL 5.3 Mon 10:30 POT 112

Improved growth of unstrained HgTe quantum well on InAs — •Mahitosh Biswas[1,2], Hartmut Buhmann[1,2], and Laurens W. Molenkamp[1,2] — [1]Institute for Topological Insulators, Universität Würzburg, 97074 Würzburg, Germany — [2]Physikalisches Institut (EP3), Universität Würzburg, 97074 Würzburg, Germany

HgTe turned out to be a prototype material for investigations of transport properties in topological insulator materials. The material system also demonstrated its versatility when compressive strain is applied, resulting in Weyl and Kane semimetal states. It has been shown that the strain can be controlled sufficiently by the period of a CdZnTe/CdTe superlattices grown on a doped GaAs substrate. However, these strained and/ or strained layers exhibit a rather high surface roughness which makes them unsuitable for sub-micrometer device fabrication or local probe measurement techniques. Here we show that CdZnTe/CdTe superlattices grown on doped InAs improve the situation significantly. Surface roughness is about three times lower compared with GaAs. These observations are confirmed by TEM measurements which monitor dislocations originating at the III-V/II-VI semiconductor interface. Magneto-transport measurements reveal that the doped substrate can be used as a highly efficient back gate. Carrier variations between $2 \times 10^{11} cm^{-2}$ (electron) and $-2 \times 10^{11} cm^{-2}$ (hole) are observed for a medium ±10 V gate range. These results manifest a (big) step forward toward the fabrication of functional top and back gated devices on topological materials.

HL 5.4 Mon 10:45 POT 112

Band alignment of thin strontium germanate layer on silicon from *ab initio* — •Tomáš Rauch[1,2], Pavel Marton[3,4], Silvana Botti[1,2], and Jiří Hlinka[3] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Germany — [2]European Theoretical Spectroscopy Facility — [3]Institute of Physics of the Czech Academy of Sciences, Praha, Czech Republic — [4]Institute of Mechatronics and Computer Engineering, Technical University of Liberec, Czech Republic

Silicon is one of the most used materials for optoelectronic applications. In photo-catalytic cells for hydrogen evolution reaction, Si must be capped by a protective layer, additionally allowing the photo-excited electrons to travel to the device surface. It has been demonstrated, that $SrTiO_3$ (STO) can fulfill these two functions [1].

In this work, we studied $SrGeO_3$ (SGO) as an alternative to STO, using density-functional theory. We calculated the structural properties of a chosen prototypical SGO/Si(001) interface and studied its electronic structure, focusing on the band offsets between Si and SGO. We found a metallic type-III interface with occupied conduction bands of SGO and a charge transfer from Si to SGO. Aligning the local band edges of the thin SGO layer with the redox potentials allows us to conclude that the SGO/Si interface should be suitable for water reduction.

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[1] Li Ji et al., Nat. Nanotechnol. **10**, 84 (2015)

HL 5.5 Mon 11:00 POT 112

Evolution of vacancy like defects in heavily doped GaAs — •Maciej Oskar Liedke[1], Slawomir Prucnal[2], Maik Butterling[1], Juanmei Duan[2], Eric Hirschmann[1], Mao Wang[2], Manfred Helm[2], Shengqiang Zhou[2], and Andreas Wagner[1] — [1]Institute for Radiation Physics, Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany — [2]Institute for Ion Beam Physics, Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany

The effect of intense pulsed laser melting and flash lamp annealing on defects distribution and activation efficiency in chalcogenide-implanted GaAs was investigated by means of positron annihilation spectroscopy and transport measurements. Using positrons as a sensitive probe of open volumes and dedicated DFT calculations, we will highlight the capability of nanosecond pulsed laser melting to control the type and density of defect complexes, e.g. S or Te substituting As atoms associated to Ga vacancy, playing a crucial role for donor deactivation. The distribution of defects and carriers will be discussed regarding the depth distribution of implanted elements and the solidification velocity during recrystallization.