HL 71: Transport Properties

Time: Thursday 9:30–11:30 Location: POT 112

HL 71.1 Thu 9:30 POT 112

Indirect excitons in (111) GaAs double quantum wells — •Colin Hubert, Alberto Hernández-Mínguez, Klaus Biermann, and Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

We study the dynamics of indirect (or dipolar) excitons (IXs) in GaAs (111) double quantum wells (DQWs) subjected to a transverse electric field. In comparison with single (111) QWs, these DQWs can store, for a comparable applied fields and optical excitation density, a density of IXs much larger than in SQWs, thus leading to stronger IX-IX repulsive interactions. We show by means of spatially-resolved optical spectroscopy that IXs in (111) DWQs can be transported over distances exceeding 60 micrometers. From the spectral dependence of the IX spatial distribution profiles, we show that the long transport distances are due to drift forces arising from the strong IX-IX interactions.

HL 71.2 Thu 9:45 POT 112

Snake-orbit induced magnetoresistance oscillations in 2D electron gases — Andreas Leuschner[1], •Jakob Schluck[1], Mihai Cerchez[1], Thomas Heinzel[1], Klaus Pierz[2], and Hans Werner Schumacher[2] — [1]Heinrich Heine University Düsseldorf, Universitätsstr. 1, D-40225 Düsseldorf — [2]Physikalisch-Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig

Localized magnetic fields of alternating sign in 2D electron gases give rise to snake- orbits. This may be realized in a Hall bar by the superposition of a homogeneous perpendicular magnetic field and a localized magnetic barrier of opposite sign [1]. The snake orbits redirect the edge states coming from source to the magnetic barrier from one edge of the Hall bar to the other, where, depending on the incident position they can be further directed back to source, or transmitted across the barrier. This has a commensurate periodic character, leading to oscillations in magnetoresistance. Experimental results and simulations are presented.

[1] S. Hugger, M. Cerchez, H. Xu, and T. Heinzel, Phys. Rev. B 76, 195308 (2007)

HL 71.3 Thu 10:00 POT 112

Thermal conductivity in intermetallic clathrates: A first-principles perspective on the phonon-glass concept — •Daniel Lindroth, Mattias Ångqvist, and Paul Erhart — Chalmers University of Technology, Department of Physics, Gothenburg, Sweden

Clathrates exhibit a very low thermal conductivity, which is a key factor for their very good thermoelectric properties and has been attributed to "phonon-glass" conduction behavior. Here, we present a computational analysis of the conduction mechanism using Ba8X16Y30 (X={Al,Ga}, Y={Si,Ge}) as model systems. Contributions to the thermal conductivity from both electrons as well as phonons are computed with Boltzmann transport theory.

The calculations are in good agreement with experimental data and in particular reproduce the experimentally observed ordering of the lattice thermal conductivity between the different systems. We demonstrate that these rather non-intuitive trends can be traced to the presence (or lack thereof) of dispersed higher frequency optical phonon modes, which provide a surprisingly large contribution to the lattice thermal conductivity. The "phonon-glass" behavior manifests itself in our calculations in the form of very short lifetimes, which indicate that already at room temperature the majority of modes is overdamped.

In terms of the electronic thermal conductivity, our results provide insight into the applicability of the Wiedemann-Franz law. While the latter is regularly used to separate lattice and electronic contributions to the thermal conductivity, our data show that the choice of pre-factor can incur an error of up to 50% for the electronic thermal conductivity.

HL 71.4 Thu 10:15 POT 112

Ab-initio phonon scattering by dislocations using Atomic-Green's function approach — •Tao Wang[1], Jesus Carrete Montaña[2], Natalio Mingo[2], and Georg K. H. Madsen[1,3] — [1]ICAMS, Bochum, Germany — [2]CEA-Grenoble, Grenoble, France — [3]Institute of Materials Chemistry, Wien, Austria

Predicting the thermal conductivity of modern semi-conductor architectures is an inherent multi-scale problem. It requires the quantification of phonon scattering strength caused by various types of defects e.g. vacancies, interfaces and dislocations, inside the materials. We introduce the atomic-Green's-function approach as an efficient way to evaluate the phonon scattering of dislocations with ab-initio precision. The three-dimensional Brillouin Zone (BZ) is divided into parallel planes perpendicular to the defect line direction. A triangulation mesh is adopted to discretize each of the two-dimensional BZ planes. By summing the Green's function results of all the linearly interpolated triangular elements on the planar sub-domains, the T-matrix and scattering cross section are obtained.

We will illustrate this strategy by setting up an atomic model of a quadrupolar arrangement of edge dislocations in silicon using linear elasticity theory. The frequency dependence of the scattering rate is calculated and discussed. Dislocation density influenced thermal conductivity evaluated from the Boltzmann-transport-equation is further analyzed to reveal how the long range elastic deformation field and short range dislocation core will modify lattice thermal transport behavior.

Coffee Break

HL 71.5 Thu 10:45 POT 112

Pressure-induced conduction band convergence in the thermoelectric ternary chalcogenide, $CuBiS_2$ — •Najebah Alsaleh, Elvis Shoko, and Udo Schwingenschlogl — King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

The pressure dependence of electronic and thermoelectric properties of four ternary chalcogenides with space group Pnma, namely, $CuSbS_2$, $CuSbSe_2$, $CuBiS_2$, and $CuBiSe_2$ are investigated up to 10 GPa by using density functional theory combined with semiclassical Boltzmann theory. The effects of Van der Waals interactions are included in all calculations since these compounds have layered structures. All the compounds have indirect band gaps which decrease monotonically with increasing pressure except for $CuBiS_2$. For this compound, an indirect-indirect band gap switching occurs around 3 GPa leading to a conduction band convergence which appears to have important implications for thermoelectric properties. From a detailed examination of the structural changes in the different compounds, the unusual properties of $CuBiS_2$ are explained.

HL 71.6 Thu 11:00 POT 112

Electron pairing in nonlinear nanoelectromechanical systems — •Matthias Droth[1], Gábor Széchenyi[2], and András Pályi[1,2] — [1]Budapest University of Technology and Economics (Budapest, Hungary) — [2]Eötvös University (Budapest, Hungary)

Despite the success of BCS-theory, the underlying mechanism for electron-pairing remains elusive for many superconducting materials. For $SrTiO_3$, it has been shown [1] that electron-pairing outside the superconducting regime can be explained with an effectively negative charging energy $U<0$. Here, we show theoretically that a quantum dot on a non-linear mechanical resonator supports electron-pair tunneling through the device by means of $U<0$ while its system parameters lie within reach of current experiments. We describe the system as a capacitor network model and discuss its relation to the Anderson-Holstein model [2]. Restricting the mechanical resonator potential to quadratic and quartic terms, we find that the system always possesses a phase that supports electron-pair tunneling. This phase can be achieved with a quantum dot on a suspended graphene resonator.

[1] Guanglei Cheng *et al.*, *Electron pairing without superconductivity*, Nature (London) **521**, 196 (2015).

[2] J. Koch, M. E. Raikh, and Felix von Oppen, *Pair tunneling through single molecules*, Phys. Rev. Lett. **96**, 056803 (2006).

HL 71.7 Thu 11:15 POT 112

Gaussian beam electron optics with quantum point contacts — •Jaan Freudenfeld[1], Sergey Platonov[1,2], Max Geier[3], Piet Brouwer[3], Vladimir Umansky[4], and Stefan Ludwig[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Deutschland — [2]Ludwig-Maximilians-Universität, München, Deutschland — [3]Freie Universität, Berlin, Deutschland — [4]Weizmann Institute of Science, Tel Aviv, Israel

Precise control of the motion of ballistic electrons on the nanoscale

would be a major step towards the realization of integrated electronic quantum circuits. Quantum point contacts (QPCs) are fundamental building blocks of nanoscale circuits and characterized by quantized conductance. The emission of electrons from these one-dimensional constrictions happens within an aperture angle and is subject to diffraction. We experimentally study the diffraction pattern of QPCs with confinement potentials resembling parabolic saddle point potentials. In contrast to usual hard wall single slit experiments our parabolic "slits" emit electrons in Hermite functions. As a consequence the ballistic electron dynamics is described by Gaussian beam electron optics yielding a very different diffraction pattern compared to the usual single slit plane wave approach. We experimentally explore the diffraction pattern by combining magnetic deflection with electrostatic focusing using a field effect lens and compare the results with model calculations. The observed diffraction pattern and focusing properties of our electrostatic lens clearly indicate Gaussian beam electron optics, a crucial information for the design of future quantum circuit applications.