# HL 36: Transport properties

Time: Thursday 9:30–11:45 Location: POT 151

HL 36.1 Thu 9:30 POT 151

**Charge carrier mobilities in 2D covalent organic frameworks** — •Elif Unsal[1], Alexander Croy[2], Alessandro Pecchia[3], Arezoo Dianat[1], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Nanotechnology, TU Dresden, Dresden, Germany. — [2]Institute of Physical Chemistry, FSU Jena, Germany. — [3]CNR-ISMN, Rome, Italy

2D COFs are functional porous crystalline structures, which have high chemical and thermal stabilities. Having tunable chemistry and structures are their major properties which make 2D COFs attractive for wide range of applications, such as electro-catalysis, gas storage, and optoelectronic applications[Xiao Feng, 2012, Chem. Soc. Rev.]. Despite the intensive studies on 2D COFs, charge transport properties of most of these materials are still unknown. Here, we present a new approach based on DFTB calculations of the phonon-limited mobility in 2D COFs. We are modelling charge transport properties by combining state-of-the-art electron-phonon coupling calculations and semiclassical Boltzmann transport theory. We are using our own code DFTBephy whose implementation is based on DFTB+ [Marcus Elstner et al. 1998, Phys. Rev. B: Condens. Matter Mater. Phys.; Marcus Elstner, 2007, J. Phys. Chem. A] and phonopy [Atsushi Togo, 2015, Scr. Mater.] and it interfaces with BoltzTrap2 [Georg K. H. Madsen, 2018, Comput. Phys. Commun.] to calculate transport properties. Our results are benchmarked against state-of-the-art EPW [Samuel Ponce, 2016, Comput. Phys. Comm.] calculations.

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**Active Dopant Sites in Hyperdoped Si and Ge Investigated by Photoemission** — •Moritz Hoesch[1], Mao Wang[2], Slawomir Prucnal[2], Shengqiang Zhou[2], Olena Fedchenko[3], Christoph Schlüter[1], Katya Medjanik[3], Sergey Babenkov[3], Anca Ciobanu[1], Dmitrii Potorochin[1,4], Sanjoy Mahatha[1,5], Markus Scholz[1], Quynh Nguyen[6], Aimo Winkelmann[7], H.-J. Elmers[3], and Gerd Schönhense[3] — [1]DESY Photon Science, Hamburg, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [3]JGU, Institut für Physik, Mainz, Germany — [4]TU Bergakademie Freiberg, Germany — [5]UGC-DAE, Indore, India — [6]SLAC, Menlo Park, USA — [7]AGH University of Kraków, Poland

Hyperdoping of silicon and germanium, with dopant concentration well above the thermal solubility limit, is achieved by ion implantation followed by pulsed laser or flash lamp annealing. Here, we probe the materials by photoemission spectroscopy thus revealing the metallic carriers in the valence region as well as core level shifts of the dopant species. The samples are p-doped Ge:Ga and n-doped Si:Te, both well into the metallic regime. The latter shows non-saturating growth of the free carrier concentration with increasing doping [1]. We present experimental determinations of the Fermi surfaces of these materials by soft x-ray ARPES as well as geometrical structure measurements by photoelectron diffraction [2,3].

[1] M. Wang et al. Phys. Rev. Appl. 11 054039 (2019). [2] O. Fedchenko et al NJP 21, 113031 (2019); [3] O. Fedchenko et al NJP 22, 103002 (2020).

HL 36.3 Thu 10:00 POT 151

**Rapid Electronic Transport Predictions via the Kubo-Greenwood Formalism** — •Florian Fiebig, Matthias Scheffler, and Christian Carbogno — The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin

For the first-principles evaluation of electronic heat and charge transport coefficients, the Kubo-Greenwood (KG) formalism [1] represents a more general and accurate alternative to perturbative approaches, [2] since it naturally incorporates all orders of anharmonic and vibronic effects. In practice, however, KG calculations come with a prohibitive computational cost, since ordered crystalline materials typically require both dense reciprocal-space **k**-grids for the electronic degrees of freedom and large real-space supercells for the vibrational ones. In this work, we propose an adaptive, KG-specific scheme for the **k**-space sampling that alleviates this issue. It enables the use of very coarse **k**-grids during the self-concistency cycle, whereas very dense **k**-grids are used for the evaluation of the KG formula, but only for those Brillouin-zone regions that contribute to the conductivities. As demonstrated for Silicon, this massively reduces the involved computational cost, and hence paves the way towards affordable, fully anharmonic predictions of electronic heat and charge transport coefficients.

[1] B. Holst, M. French, and R. Redmer, *Phys. Rev. B* **83**, 235120 (2011).
[2] S. Poncé, E. R. Margine, and F. Giustino, *Phys. Rev. B* **97**, 121201 (2018).

HL 36.4 Thu 10:15 POT 151

**Semiconductor to Semimetall Transition in Bi-based Core-Shell Nanowires** — Maximilian Kockert[1], Rüdiger Mitdank[1], Mahni Müller[1], Hongjae Moon[2], Jongmin Kim[2], Wooyoung Lee[2], and •Saskia Fischer[1] — [1]Humboldt-Univ. zu Berlin, Germany — [2]Yonsei Univ., Seoul, Korea

The full-thermoelectric characterization of individual core/shell Bi-based nanowires is presented. Compressive strain induced by a $TiO_2$ shell can lead to a band opening increasing the absolute Seebeck coefficient by up to 30 percent compared to bulk at room temperature [1]. If the strain exceeds the elastic limit the semimetallic state is recovered due to the lattice relaxation. The influence of strain on the temperature dependence of the electrical conductivity, the absolute Seebeck coefficient and the thermal conductivity of bismuth/titanium dioxide ($Bi/TiO_2$) nanowires with different diameters was measured and compared to bismuth (Bi) and bismuth/tellurium (Bi/Te) nanowires and bismuth bulk. Different nano-contacting methods are discussed.

[1] M. Kockert, *et al.*, Nanoscale Advances **3** (2021) 263

**30 min. break**

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**Comprehensive model for the thermoelectric properties of two-dimensional carbon nanotube networks** — •Aditya Dash, Dorothea Scheunemann, and Martijn Kemerink — Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany.

Networks of semiconducting single-walled carbon nanotubes (SWCNTs) are interesting thermoelectric materials due to the interplay between CNT and network properties. Here we present a unified model to explain the charge and energy transport in SWCNT networks. We used the steady-state master equation for the random resistor network containing both the intra- and inter-tube resistances, as defined through their 1D density of states that is modulated by static Gaussian disorder. The tube resistance dependence on the carrier density and disorder is described through the Landauer formalism. Electrical and thermoelectric properties of the network were obtained by solving Kirchhoffs laws through a modified nodal analysis, where we used the Boltzmann transport formalism to obtain the conductivity, Seebeck coefficient, and electronic contribution to the thermal conductivity. The model provides a consistent description of previously published experimental data for temperature and carrier density-dependent conductivities and Seebeck coefficients, with energetic disorder being the main factor explaining observed mobility upswing with carrier concentration. For lower disorder, the Lorentz factor obtained from simulation is in accordance with the Wiedemann-Franz law. Suppressed disorder and lattice thermal conductivity can be a key to higher zT.

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**Thermal mapping of a c-plane oriented GaN membrane** — •Mahmoud Elhajhasan[1], Isabell Hüllen[1], Wilken Seemann[1], Jean-François Carlin[2], Ian Rousseau[2], Nicolas Grandjean[2], and Gordon Callsen[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Institute of Solid State Physics, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

The thermal characterization of modern semiconductor membranes commonly employed for photonic devices like nanobeam lasers (1D) or photonic crystals (2D), often lacks spatial resolution and appropriate quantification of local temperatures. However exactly these two points are relevant for the detection of e.g., thermal anisotropies, heat leakage, and interfaces providing thermal resistance.

In this contribution, Raman thermometry employing one laser beam (1LRT) is used to quantify the thermal conductivity $\kappa$ of 250-nm-thick, state-of-the-art, c-plane wurtzite GaN membranes. The same mem-

branes are then probed by two laser Raman thermometry (2LRT) to map the temperature distribution caused by a heating laser via a second probe laser. From such a map, $\kappa$ is extracted for all in-plane crystal directions, yielding a thermal anisotropy in the c-plane of GaN. Comparing this direct, sub-$\mu$m spatially resolved imaging technique to classical Fourier simulations reveals a significant divergence at the heating laser spot pointing to non-diffusive phonon transport.

In conclusion, our comparison of 1LRT and 2LRT measurements provides insight into the applicability of each technique to determine the thermal conductivity of photonic membranes.

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**Tunable preferable orientation of $\alpha$-FeSi2 crystallites on silicon surfaces** — •Tatiana Smoliarova, Ivan Tarasov, and Ulf Wiedwald — Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057, Duisburg, Germany

Nowadays, one of the most important applications of silicon (Si) and Si-based functional materials is microelectronics. Silicon forms compounds in the form of solid solutions or intermetallic compounds * silicides. Metallic $\alpha$-FeSi2 phase can be used as a contact material to silicon or to the semiconducting $\beta$ FeSi2 phase with good ohmic characteristics.

In this work, we discuss the growth of $\alpha$-FeSi2 submicron-size crystallites on gold-activated and gold-free p-Si(001), p-Si(110) and p-Si(111) surfaces via molecular beam and reactive epitaxy. The study reveals that the surfactant-assisted mediated epitaxy regulates morphology and the preferable orientation relationship (OR) of the crystallites to Si. According to the X-ray diffraction, strongly preferable ORs are $\alpha$-FeSi2(001)//Si(001), $\alpha$-FeSi2(001)//Si(111), $\alpha$-FeSi2(001)//Si(110) for gold-activated and $\alpha$-FeSi2(111)//Si(001), $\alpha$-FeSi2(211)//Si(110), $\alpha$-FeSi2(112)//Si(111) for gold-free Si substrates. Thus, the orientation control of fabricated $\alpha$-FeSi2 crystallites can be used for tuning electron transport across the metal/semiconductor interface.

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