HL 23: Transport Properties

Time: Wednesday 9:30–12:15 Location: POT/0051

HL 23.1 Wed 9:30 POT/0051

Nonlinear charge transport in single crystalline slabs of Bi2Se3 — •Igor Veremchuk[1], Pavlo Makushko[1], Anita Guarino[2], Muhammad Waqee Ur Rehman[2], Rosalba Tatiana Fittipaldi[2], Tobias Kosub[1], Alexej Pashkin[1], Fabian Ganss[1], Proloy T. Das[1], Rui Xu[1], Rhonald Burgos Atencia[3], Debottam Mandal[3], Antonio Vecchione[2], Carmine Ortix[3,2], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany — [2]CNR-Institute for SuPerconductors, Innovative materials, and devices, Salerno, Italy — [3]Dipartimento di Fisica "E. R. Caianiello", Universita di Salerno, IT-84084 Fisciano (SA), Italy

Nonlinear charge transport is central to next-generation high-frequency electronics, enabling efficient rectification and frequency conversion up to the THz range. Nonlinear responses are observed in various material systems often focusing on thin films including Bi [1], Te [2], and Bi2Se3 [3]. In this study, we will report experimental observations of nonlinear charge transport in Bi2Se3 single crystals, which is explained based on peculiarities of the structural properties of layered Bi2Se3 materials. Our findings can be applied to a broad range of van der Waals centrosymmetric compounds.

[1] P. Makushko, I. Veremchuk et al., Nat. Electron. 7, 207 (2024).
[2] B. Cheng et al., Nat. Commun. 15, 5513 (2024).
[3] P. He et al., Nat. Commun. 12, 698 (2021).

HL 23.2 Wed 9:45 POT/0051

Comparing thermal conductivity predictions from open source phonon transport solvers — •Sally Issa, Martí Raya-Moreno, and Nakib H. Protik — Humboldt-Universität zu Berlin, Germany

Phonon transport continues to be an active field of research, both for probing materials physics and developing applications for thermoelectricity and thermal management. Due to their parameter-free nature, ab initio approaches are one of the preferred means for solving the phonon transport problem, offering excellent predictive capabilities, especially for novel materials. Over the last decade, the workflow combining density functional theory (DFT) and the Peierls Boltzmann transport equation (BTE) has gained popularity. Indeed, practitioners in the field have several publicly available BTE code packages to choose from, for example, ShengBTE, AlmaBTE, phonop3py, elphbolt, Phoebe, etc., that use this workflow. Nevertheless, the doubt regarding the comparability of these different codes still remains. At present, a detailed comparative study is missing in the literature. In this work, we fill this gap and carry out a comparison of the phonon thermal conductivity predicted by various codes. For a fair comparison, we use the same DFT generated interatomic force constants from the Alma database [1] for all considered codes. We carefully check the convergence of the thermal conductivity with respect to the wave vector mesh density and compare the results over a range of temperature points.

[1] ALMA database: https://almabte.bitbucket.io/database/

HL 23.3 Wed 10:00 POT/0051

Influence of Thermal Annealing on CMOS-Integrated Graphene Field-Effect Transistors — •Daniel Nickel[1], Daniele Capista[1], Rasuole Lukose[1], Christian Wenger[1,2], and Mindaugas Lukosius[1] — [1]IHP - Leibniz Institute for High Performance Microelectronics, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]BTU Cottbus Senftenberg, Platz der Deutschen Einheit 1, 03046 Cottbus, Germany

This work investigates the influence of consecutive annealing on CMOS-integrated graphene field-effect transistors (GFETs) with annealing temperatures (T_a) from 150 °C up to 300 °C. The GFETs were fabricated on 200 mm SiO_2/Si wafers with Pd/Au and Ni edge contacts, tungsten backgate and Si_3N_4 passivation. Annealing was carried out in 150 sccm nitrogen flow for 1 h using a 10 °C/min ramp. Electrical transfer measurements show that maximum p- and n-type field-effect mobilities occur at T_a = 200 °C for Pd/Au ($\mu_p \approx 950$ cm^2/Vs, $\mu_n \approx 1650$ cm^2/Vs) and at T_a = 150 °C for Ni ($\mu_p \approx 450$ cm^2/Vs, $\mu_n \approx 890$ cm^2/Vs). Raman analysis indicates an improved graphene quality with increasing T_a. Raman mapping reveals that for Pd/Au, the FWHM of the 2D peak reaches a minimum at T_a = 200 °C, followed by a slight increase in compressive strain at higher T_a. For Ni, broader 2D and G peak distributions and a reduction in p-doping with increased T_a is observed. Raman data measured near the Ni contacts reveal reduced p-doping, whereas doping near the Pd/Au contacts remains largely unaffected. Funding was provided by EU Horizon 2020 Graphene Flagship grants 101189797 and 101120938.

HL 23.4 Wed 10:15 POT/0051

Elucidating mobile charge carriers in granular matter by transient surface photovoltage analysis — •Christoph Merschjann[1], Albert These[2], Christoph Brabec[2,3], Thomas Dittrich[1], and Pablo Jimenéz-Calvo[2,4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen — [3]Helmholtz-Institute Erlangen-Nürnberg, Erlangen — [4]Max-Planck-Institute of Colloids and Interfaces, Potsdam

Among the most important properties of novel functional materials are their charge transport characteristics, including n vs. p type conductivity, carrier concentrations, and respective mobilities. However, new solid-state materials are typically first synthesized in granular form, and often this is also the intended morphology for applications (batteries, photocatalysts, etc.). This makes most electrical characterization techniques (e.g. impedance, Hall, time-of-flight photocurrent) extremely challenging, as they rely on current measurements throughout the bulk of the sample. To overcome this drawback, we use contactless transient surface photovoltage (TR-SPV) to detect charge-density shifts on the nanometer scale and in a time range from nanoseconds to seconds. Comparing the results with diffusive charge-transport models of moderate complexity, we are able to deduce the type and mobility of photoinduced charge carriers in a prominent example material, graphitic polymeric carbon nitride (PCN). We encourage transferability of this SPV analysis to other 2D layered systems like metal- or covalent-organic frameworks (MOF / COF).

HL 23.5 Wed 10:30 POT/0051

Deep-learning Hamiltonian Acceleration of Electrical Transport Predictions using the Non-Perturbative *ab initio* Kubo-Greenwood Method for Strongly Anharmonic Materials — •Juan Zhang[1,2], Kisung Kang[3], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the FHI of the Max Planck Society, Berlin — [2]Department of Optical Science and Engineering, Fudan University, Shanghai — [3]School of Materials Sciences and Engineering, Chonnam National University, Gwangju

Thermal insulators, e.g., needed for efficient thermoelectric materials, feature strong anharmonicity. As a consequence, a perturbative approach of electron-phonon interactions and even the phonon concept for describing vibrations may become invalid. The non-perturbative *ab initio* Kubo-Greenwood (aiKG) method provides an approach for evaluating electron and hole mobilities [1]. However, it requires substantial computational costs due to its high requirements with respect to statistical averages, large supercells, and extrapolation strategies to the zero-frequency limit. This work introduces an AI-assisted aiKG framework for the FHI-aims code, which incorporates the neural-network model, DeepH [2], trained to predict the Kohn-Sham Hamiltonian. Using the thermal insulator KI, we demonstrate the capabilities and predictive power of the approach, which substantially accelerates the calculation of large supercell electronic band structures, temperature-dependent spectral functions, and carrier mobilities with high accuracy.

[1] J. Quan *et al.* Phys. Rev. B 110, 235202 (2024).
[2] X. Gong, *et al.* Nat Commun 14, 2848 (2023).

HL 23.6 Wed 10:45 POT/0051

Quantum oscillations in the correlated metal $CaVO_3$ — Olivio Chiatti[1], Mahni Müller[1], Maria Espinosa[1], Tatiana Kuznetsova[2], Roman Engel-Herbert[2,3], and •Saskia F. Fischer[1,4] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, USA — [3]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin, Germany — [4]Center for the Science of Materials Berlin, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Transparent conductive materials are in great demand in the opto-

electronic industry for their high-performance and cost-effectiveness. Strong electron-electron interactions in correlated metals can enhance the carrier effective mass and allow to achieve both high-optical transparency and high-electrical conductivity [1].
Here, we study the electric transport properties of thin $CaVO_3$ epitaxial films grown on $LaAlO_3$ substrates by hybrid molecular beam epitaxy, with residual a high resistivity ratio (RRR) up to 98 [2]. Magnetortransport measurements were performed between 2 and 200 K in magnetic fields up to 64 T. Films with high RRR show quantum oscillations below 10 K. The analysis of the Shubnikov-de Haas oscillations provides parameters within a multi-carrier model and the implications for the complex Fermi surface of $CaVO_3$ are discussed.
[1] Zhang *et al.*, Nature Materials **15**, 204 (2016)
[2] Kuznetsova *et al.*, APL Materials **11**, 041120 (2023)

15 min. break

HL 23.7 Wed 11:15 POT/0051

Modeling the impact of dynamic disorder on optical conductivity of semiconductors using a Kubo approach — •Frederik Vonhoff[1], Michel Panhans[2], David R. Reichman[3], Frank Ortmann[2], and David A. Egger[1] — [1]Physics Dep., TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [2]Dep. of Chemistry, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [3]Dep. of Chemistry, Columbia University, New York, NY 10027, USA

Semiconductor devices rely critically on efficient charge-carrier transport, making it essential to understand the underlying transport mechanisms. The optical conductivity is a key transport observable, both experimentally and theoretically, for identifying the scattering mechanisms and transport regimes. However, modeling the transport properties of semiconductors with strong nuclear vibrations is challenging due to the resulting dynamic disorder in the electronic structure [1, 2]. Addressing these challenges, we develop a dynamic-disorder-driven microscopic method to compute optical conductivities in one- and three-dimensional semiconductor model systems by integrating time-dependent electronic Hamiltonians in Kubo transport theory. By systematically varying the static and dynamic disorder strength, we investigate the transition from localization to transient localization to and diffusive behavior, providing insights into scattering mechanisms active in emerging semiconductor materials such as halide perovskites.
[1] J. Fetherolf, et al, Physical Review X 10, 021062 (2020)
[2] F. Vonhoff, et al, Physical Review Materials 9, 094601 (2025)

HL 23.8 Wed 11:30 POT/0051

Self-Trapped Exciton Diffusion in a Lead-Free Two- Dimensional Hybrid Perovskite — •Jan-Heinrich Littmann[1], Lukas Gümbel[1], Philip Klement[1], Meng Yang[2], Markus Stein[1], Johanna Heine[2,3], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]Department of Chemistry and Material Sciences Center, Philipps-Universität Marburg, Hans-Meerwein- Straße, 35043 Marburg, Germany — [3]Institute of Chemistry, Carl von Ossietzky Universität Oldenburg, Ammerländer Heerstraße 114-118, 26129 Oldenburg, Germany

Self-trapped excitons (STEs) in low-dimensional metal-halide perovskites arise from lattice distortions. The mobility of such excitations is expected to be limited, however, remains vastly unexplored experimentally.

Here, we directly image STE transport in a lead-free perovskite using spatially and temporally resolved photoluminescence microscopy. The STEs exhibit measurable mobility and propagate over micrometer distances despite their strongly-localized nature. At low temperatures, their motion is limited and nearly temperature independent. Transport becomes thermally activated above 150k and overcomes local energy barriers. Together this infers trap-limited diffusion. These results establish that STEs are mobile under suitable conditions and provide a quantitative framework for STE transport in lead-free perovskite materials.

HL 23.9 Wed 11:45 POT/0051

Electron-phonon interactions in VASP — •Manuel Engel[1], Henrique Miranda[1], Atsushi Togo[2], Laurent Chaput[3], Martijn Marsman[1], and Georg Kresse[1,4] — [1]VASP Software GmbH, Vienna, Austria — [2]National Institute for Materials Science, Tsukuba, Japan — [3]Lorraine University, Nancy, France — [4]University of Vienna, Vienna, Austria

Understanding electron-phonon interactions with first-principles accuracy is essential for predicting temperature-dependent electronic properties in semiconductors and complex materials. In this work, we present new capabilities implemented in VASP that enable a fully ab initio treatment of electron-phonon coupling using the projector-augmented wave (PAW) method. These developments provide a consistent framework for evaluating band-gap renormalization, phonon-induced linewidths, and finite-temperature electronic transport properties within density functional theory.

Our approach combines perturbative electron-phonon matrix elements with dense Brillouin-zone sampling achieved through interpolation techniques compatible with PAW-based orbitals and higher-level density functionals. We demonstrate accurate predictions of zero-point and thermal band-gap shifts across a range of materials. In addition, we incorporate the electron-phonon scattering rates directly into Boltzmann transport calculations under relaxation-time approximations. This enables temperature-dependent mobilities and conductivities to be computed from first principles.

HL 23.10 Wed 12:00 POT/0051

Investigation of exciton diffusion in GaAs nanowires via cathodoluminescence spectroscopy — •Mikel Gómez Ruiz, Vladimir Kaganer, Jesús Herranz, Lutz Geelhaar, Oliver Brandt, and Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

Semiconductor nanowire (NW) structures emitting at tailored wavelengths have attracted notable interest for integration with silicon-on-insulator waveguides. For many of these applications, the efficiency with which carriers are injected into the active region of the sample is relevant.

In this context, carrier transport in phase-pure GaAs nanowires is investigated by spatially-resolved cathodoluminescence spectroscopy. Emission intensity profiles along the nanowire axis are measured to study carrier transfer from the GaAs segment to the axial interfaces at both ends of the nanowire. These interfaces are formed at the top with the axially grown (Al,Ga)As shell and at the bottom with the Si substrate. The recorded intensity profiles are predominantly asymmetric, indicating that carrier recombination at the two interfaces occurs in a different fashion.

These profiles are analyzed using a mathematical model that accounts for carrier generation, diffusion, and recombination. Fitting this model to the experimental profiles reveals a diffusion length exceeding one micron at 10 K, an unprecedented value for GaAs nanowires. This reflects the high crystal quality of our nanowires.