HL 7: Transport properties I

Time: Monday 15:00–17:00 Location: ER 325

HL 7.1 Mon 15:00 ER 325

Challenges of mapping transport parameters of N-doped 4H-SiC by Raman spectroscopy — •Hannes Hergert[1,2], Matthias T. Elm[1,2,3], and Peter J. Klar[1,2] — [1]Center for Materials Research, Giessen, Germany — [2]Instituten of Experimental Physics I, Giessen, Germany — [3]Institute of Physical Chemistry, Giessen, Germany

We assess Raman spectroscopy as a tool for fast and non-invasive mapping of charge carrier density and carrier mobility in inhomogeneously doped 4H-SiC. For this purpose, we compare values of these transport parameters obtained by magneto-transport and Raman measurements of N-doped 4H-SiC. The effective charge density and mobility, which are obtained from resistivity and Hall measurements by employing the commonly used effective one-band model, deviate from the values extracted by applying the established line-shape models for describing the longitudinal optical phonon coupled (LOPC) modes in the Raman spectra. Differentiating between free and localized carriers in the framework of a three-band transport model confirms that only the free charge carriers in the conduction band of N-doped 4H-SiC contribute to the LOPC Raman signal and their density agrees well with that obtained by the line shape analysis. The agreement of the mobility values is reasonable keeping in mind that different frequencies of the applied electric fields are used in the two approaches. Moreover, the excitation of electrons into the conduction band by the laser causes differences in the temperature dependence of the carrier density compared with the electrical transport data.

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Stoichiometry fluctuations and geometrical confinement in random alloys: a case study on SiGe:C — •Daniel Dick[1,2,3], Florian Fuchs[1,2,3], Jörg Schuster[1,2,3], and Sibylle Gemming[3,4] — [1]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Insitute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [3]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany — [4]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany

We investigate the effect of base layer scaling in silicon-germanium (SiGe) heterojunction bipolar transistors (HBTs) and evaluate the effect of local fluctuations in atomic concentrations using electronic structure theory.

For calculating the band structure of SiGe:C alloy with varying Ge and C content we present a new parameterization of Germanium in the framework of extended Hückel theory (EHT). Combined with the use of empirical potentials for structural relaxation, it enables us to efficiently simulate a large number of permutations of the atomic structure to quantify the influence of atomic-scale fluctuations on the electronic structure and transport properties using unit cells with more than a hundred atoms.

Comparing bulk SiGe:C alloy and thin layers gives insight on how quantum confinement and local stoichiometry fluctuations affect transport properties of ultra-scaled HBTs. Results are verified by first-principles calculations using density functional theory.

HL 7.3 Mon 15:30 ER 325

Ti_2MnAl and its modifications, as possible Spin-Gapless-Semiconductor materials. — •Jerzy Goraus, Wojciech Gumulak, and Jacek Czerniewski — Institute of Physics, Faculty of Science and Technology , University of Silesia, 41-500 Chorzów, 75 Pułku Piechoty 1A, Poland

Ti_2MnAl was earlier predicted to exhibit Spin-Gapless-Semiconductor (SGS) properties. SGS materials are very interesting due to their potential applications in spintronics. Only in one variant of crystal structure, Ti_2MnAl can have such properties; this variant (as we and other researchers have already shown) is not realized in nature. There were, however, papers claiming that element substitution of Ti_2MnAl could stabilize inverse Heusler structure for which SGS state is possible. In that presentation, we report our results for studies of Ti_2MnAl where Al was substituted by In or Sn, as well as for the isoelectronic $Ti_2Fe_{0.5}Cr_{0.5}Al$ compound. We show the results of our experimental measurements - polycrystalline samples characterized with XRD technique, with their resistivity and magnetic properties measurements as well as DFT calculations of the stability of the particular unit cell. We will also show these results in the context of our earlier research of similar materials involving sample surface measurements such as XPS and XAS measurements. The latter, as shown in our earlier report for Ti_2CrAl can also resolve the unit cell structure, which is difficult for these materials by the XRD technique alone.

HL 7.4 Mon 15:45 ER 325

Electrical Conductivity and Carrier Mobility for Strongly Anharmonic Materials from First Principles — •Jingkai Quan[1,2], Christian Carbogno[1], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195, Berlin, Germany — [2]Max-Planck Institute for the Structure and Dynamics of Matter, Luruper Chausse 149, 22761, Hamburg, Germany

First-principle approaches for describing phonon-limited electronic transport are typically based on many-body perturbation theory and the Boltzmann transport equation, which can be questionable in strongly anharmonic systems. Combining ab initio molecular dynamics (aiMD) simulations and the Kubo-Greenwood (KG) formalism, we investigate a non-perturbative stochastic method to calculate carrier mobilities, which accounts for all orders of anharmonic and vibronic couplings. We implement the KG formula in the highly efficient all-electron code FHI-aims. In particular, we discuss in this talk the definition of carrier mobility in the KG framework and the developed numerical strategies employed to overcome the notoriously slow convergence of the phase-space and Brillouin-zone integrals in crystalline solids. Using strongly anharmonic perovsktie $SrTiO_3$ and $BaTiO_3$, we demonstrate the capabilities and predictive power of the KG approach and investigate the influence of the chosen exchange-correlation functional on the obtained conductivities and mobilities. Eventually, we analyze the observed trends and explain the effects in terms of self-energy shifts and broadenings.

15 min. break

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Electronic Transport Properties of Janus Ge-Based Two-Dimensional IV-V Monolayer — •Dogukan Hazar Ozbey[1], Gozde Ozbal Sargin[2], Veli Ongun Ozcelik[2], and Engin Durgun[1] — [1]Bilkent University UNAM — [2]Sabanci University

Two-dimensional (2D) semiconductors with anisotropic properties have garnered significant attention in materials research, particularly those exhibiting strong anisotropy in carrier mobility. A captivating subset of these materials is Janus monolayers, characterized by the substitution of all atoms on one side of their binary counterpart with a different element. This structural transformation disrupts the out-of-plane mirror symmetry, offering a platform for exploring extraordinary physical properties in 2D Janus crystals. In this study, we present a comprehensive exploration of the electronic transport properties of a Janus Ge-based 2D IV-V monolayer. Our investigation employs density functional theory in conjunction with the non-equilibrium Green's function approach. To characterize the current-voltage (I-V) characteristics of the monolayer, we establish a two-probe system with the intrinsic 2D monolayer serving as channel and doped monolayer as electrodes. We systematically investigated the effect of the doping concentration of the probes and channel length on the transport properties. Our results demonstrate that this Janus monolayer displays unique transport characteristics, including a direct bandgap and carrier mobility that depend on the lattice direction, indicating anisotropic transport behavior. These unique characteristics position the monolayer as a promising candidate for applications in the field of nanoelectronics.

HL 7.6 Mon 16:30 ER 325

Charge Carrier Mobilities in 2D Carbon Allotropes — •Elif Ünsal[1], Alexander Croy[2], Alessandro Pecchia[3], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Dresden, Germany — [2]Institute of Physical Chemistry, Friedrich-Schiller-Universität, Jena, Germany — [3]CNR-ISMN, Monterotondo Stazione, Rome, Italy

Calculation of electron-phonon couplings from first principles is computationally very challenging and remains mostly out of reach particu-

larly for systems with a large number of atoms. Semi-empirical methods, like DFTB, offer a framework to obtain quantitative results at reasonable computational costs. Herein, we are modelling charge transport properties by combining state-of-the-art electron-phonon coupling calculations and semi-classical Boltzmann transport theory. We are using our own code DFTBephy [Croy et al. J. Comput. Electron., 2023] whose implementation is based on DFTB+ [Elstner et al, Phys. Rev. B, 1998] and phonopy [Togo et al, Scr. Mater., 2015] and it interfaces with BoltzTrap2 [Madsen et al., Comput. Phys. Commun., 2018] to calculate transport properties. Our results are bechmarked against state-of-the-art EPW [Poncé et al., Comput. Phys. Comm., 2016] calculations. As a test case, we focused 2D carbon allotropes like graphyne and graphdiyne, and investigated the mechanisms underlying carrier scattering and mobilities within these materials. Our results align with the literature, affirming that the DFTBephy method gives consistent results.

HL 7.7 Mon 16:45 ER 325

Superconductivity and the normal state quantum geometry in two-dimensional superconductors — •Florian Simon, Louis Pagot, Marc Gabay, and Mark-Oliver Goerbig — Laboratoire de Physique des Solides, Université Paris-Saclay, Orsay, France

Superconductivity has, since 1911, become a pillar and a flagship of condensed matter physics. The main paradigm is given by BCS theory which, in its standard form, consists of quasiparticles in a single, partially filled band, pairing and thus condensating in a collective dissipationless state. This single band approximation has its limits. Indeed, since the 1980s, physicists have come to realize that in a multiband setting, even adiabatic, each band will carry an influence of the other bands in the form of two geometric quantities, namely the Berry curvature and the quantum metric. These quantities form what we call band/quantum geometry. In the context of superconductivity, this means that even if a single band is involved in the Cooper pairing, it can carry a quantum geometry if the normal state (NS) has more than one band. The influence of this NS quantum geometry on the superconducting state is the subject of this talk. On one side, we study the influence of the NS Berry curvature on BCS theory in the context of two-dimensional massive Dirac fermions. We find that it generally lowers the critical temperature, in a quantifiable way. On another side, we consider the two-dimensional (111) $LaAlO_3/SrTiO_3$ interface. Our results suggest that the quantum metric has a sizeable role in the appearance of superconducting domes in this interface, as a function of gate voltage.