# MM 24: Transport in Materials: Diffusion, Conduction of Charge or Heat II

Time: Tuesday 11:45–13:15 Location: C 264

MM 24.1 Tue 11:45 C 264

**Towards Highly Conductive Graphite Films: Tungsten Carbide Doping of Thermally Reduced Graphene Oxide Paper** — •Leonhard Niemann[1,2], Tianshan Xu[1,3], Markus Gruschwitz[2], Martin Köhne[1], and Christoph Tegenkamp[2] — [1]Robert Bosch GmbH, Department of Advanced Technologies and Micro Systems, 71272 Renningen — [2]Technical University of Chemnitz, Institute of Physics, 09107 Chemnitz — [3]RWTH Aachen, Gemeinschaftslabor für Elektronenmikroskopie GFE, 52062 Aachen

The growth of consumer electronics and the electrification of transport has increased enormously the demand for copper. This will lead to a global shortage of this element. Graphene-based conductors are an interesting lightweight and low-cost alternative. However, the electrical conductivity values achieved to date are not sufficient to compete with traditional copper-based conductors. To increase the electrical conductivity, various additives are under research. This study delves into the synergistic effects of tungsten carbide (WC) doping on the graphitization process of graphene oxide (GO) films. Tungsten, a well-known catalyst for promoting graphitization in amorphous carbon structures, holds promise for advancing the properties of graphene-based materials. We focused on optimizing the concentration of W to facilitate the graphitization of GO films. The samples were subjected to controlled thermal treatments, and their structural evolution was characterized. The resulting WC/graphite films with a conductivity of 432 to 594 kS/m demonstrate a concentration-dependent effect, with an optimal concentration range of 1 to 3 $\mu$mol/mg of $WS_2$ in GO.

MM 24.2 Tue 12:00 C 264

**Charge transport simulation using kinetic Monte Carlo with fast update rules** — •Roya Ebrahimi Viand, Karsten Reuter, and Sebastian Matera — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The diffusion of particles in a solid material is often characterized by rare jumps between low-energy sites, which allows for the simulation of long-time dynamics using the kinetic Monte Carlo (kMC) methodology. In the case of charged particles, kMC can become costly because the long-range Coulomb interaction requires recalculating all process rates in every kMC step, despite the fact that each step introduces only local changes in the system's state. In this talk, we introduce update rules for, in general, anisotropic lattices, which require only two element-wise vector multiplications. This can be implemented very efficiently on modern compute architectures, and we discuss this using a newly developed kMC framework. We demonstrate the approach on a first-principles kMC model for $Li^+$ transport in graphite in a high state of charge and investigate the dependence of mobility on the charge carrier density.

MM 24.3 Tue 12:15 C 264

**Chiral anomaly induced monopole current and nonlinear circular dichroism** — •Nikolai Peshcherenko[1], Claudia Felser[1], and Yang Zhang[2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187, Dresden, Germany — [2]University of Tennessee, Knoxville, Tennessee 37996, USA

Topological Weyl and Dirac semimetals are known to demonstrate a chiral anomaly effect subject to parallel electric and magnetic fields. The most well-known experimental probe of this effect is large negative longitudinal magnetoresistance. However, due to other strongly non-isotropic contributions to magnetoresistance existing in semimetals it could be interesting to consider other possible types of chiral anomaly experimental manifestations.

We suggest a simple chirality probe in TR invariant Weyl and Dirac semimetals with nonlinear Hall response. We demonstrate that chiral anomaly-induced relative shift of Weyl cones in energy space gives rise to chirality-asymmetric intranode momentum relaxation times. Due to this asymmetry, proportional to anomalous velocity Hall currents excited by external electric fields in different Weyl nodes do not perfectly compensate each other. We predict that this effect could be also observed in circular dichroism measurements.

MM 24.4 Tue 12:30 C 264

**spin Hall effect in antiferromagnetic alloys** — •Nabil Menai[1], Martin Gradhand[1], and Derek Stewart[2] — [1]University of Bristol, Bristol, UK — [2]Western Digital Research Center, San Jose, CA, USA

Historically, antiferromagnets (AFM) were believed not to exhibit any anomalous Hall conductivity (AHC). Conversely, ferromagnets have been known for a long time to show a transverse voltage without the need for a magnetic field. Very recently, however, it was shown that some AFMs can indeed manifest AHC. Furthermore, AFMs could serve as a promising component for next-generation spintronics devices, thanks to their scalability, robustness against external magnetic fields, and ultrafast spin dynamics.

In this work, we employ density functional theory and Green function methods to calculate the transport properties of Mn based binary alloyed AFMs, specifically focusing on the spin Hall conductivity (SHC). Our goal is to identify a suitable AFM for spintronic applications that exhibits a high spin Hall angle (SHA).

Our findings indicate that doping MnPt with Pd can increase the SHA from around 2% to 5%. This enhancement should be experimentally observable, particularly at room temperature where the effect is further amplified, resulting in the SHA reaching around 8%. Additionally, we present examples of AFM materials in which non-symmorphic symmetries give rise to topological features such as the emergence of Dirac nodal lines, or even a new magnetic phase termed altermagnetism. These nodal lines have been shown to substantially enhance the SHC, offering potential applications in the field of spintronics.

MM 24.5 Tue 12:45 C 264

**Exploring the tunability of the electronic properties of ZrSiSe** — •Davide Pizzirani[1,2], Oleksandr Zheliuk[1,2], Julia Kreminska[3], Pim van den Berg[1,2], Claudius Müller[1,2], Maarten van Delft[1,2], Ratnadwip Shinga[4], Yu-Te Hsu[1,2], Leslie Schoop[4], Justin Ye[3], Nigel Hussey[1,2,5], and Steffen Wiedmann[1,2] — [1]HFML-FELIX, Radboud University, 6525 ED Nijmegen, the Netherlands. — [2]Institute for Molecules and Materials, Radboud University, Nijmegen 6525AJ, the Netherlands. — [3]Device Physics of Complex Materials, Zernike Institute for Advanced Materials, Nijenborgh 4, 9747 AG, Groningen, the Netherlands. — [4]Department of Chemistry, Princeton University, Princeton, NJ 08544, USA. — [5]H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, United Kingdom.

The interplay of topology and electronic correlations, as well as the transport properties of charge carriers with a linear dispersion, can be unraveled in nodal line semi-metals, such as ZrSiSe. We present thickness- and gate-dependent magneto-transport experiments up to 35 T on exfoliated high-quality thin flakes of ZrSiSe, with sample thicknesses ranging from 112 to 27 nm. In order to further investigate the tunability of the charge carrier properties in ZrSiSe, we additionally employ the ionic-liquid gating technique. As a function of thickness and applied gate voltage, we observe strong deviation from the quadratic magneto-resistance expected for compensated semimetals as well as an alteration of the Fermi surface, evidenced by a shift in the quantum oscillation spectra.

MM 24.6 Tue 13:00 C 264

**Violation of Boltzmann quasi-particle transport in disordered alloy** — •Gabor Csire[1], Franco Moitzi[1], Andrei Ruban[1,2], and Oleg Peil[1] — [1]Materials Center Leoben Forschung GmbH, Roseggerstraße 12, 8700 Leoben, Austria — [2]KTH Royal Institute of Technology, Brinellvagen 23, SE-100 44 Stockholm, Sweden

High resistivity disordered metals often exhibit deviations from the transport behavior described by the semiclassical Boltzmann theory. Here the scattering events from impurities or phonons cannot be treated as independent processes as suggested by Matthiessen's rule. The most extreme example of such a behavior are crystalline metallic alloys that exhibit a crossover from the positive to negative sign of the temperature coefficient of resistivity that persists from low to high temperatures. Various mechanisms, including weak localization and polaronic effects, have been put forward to explain the behavior within the framework of the Boltzmann transport theory but since most of these studies were relying on simple models a clear physical picture and quantitative material-specific description are still missing. In this contribution, we investigate the temperature-dependent resistivity of such „anomalous" alloys using our recent implementation of

the Kubo-Greenwood formalism within the Korringa-Kohn-Rostoker method using Andersen's muffin-tin-orbital representation. In particular, we examine the temperature evolution of the non-Boltzmann transport contributions and discuss the origin of the sign change in the temperature coefficient.